Supplementary material

Modeling the influence of carbon branching structure on SOA formation via multiphase reactions of alkanes

Azad Madhu[1], Myoseon Jang[1], and Yujin Jo[1]

[1]Engineering School of Sustainable Infrastructure and Environment, University of Florida, Gainesville, 32608, United States of America

Correspondence to: Myoseon Jang (mjang@ufl.edu)

This file includes:
5 Tables
3 Figures
References

Section S1. Comparison of autoxidation between heptamethyl-nonane and n-C16

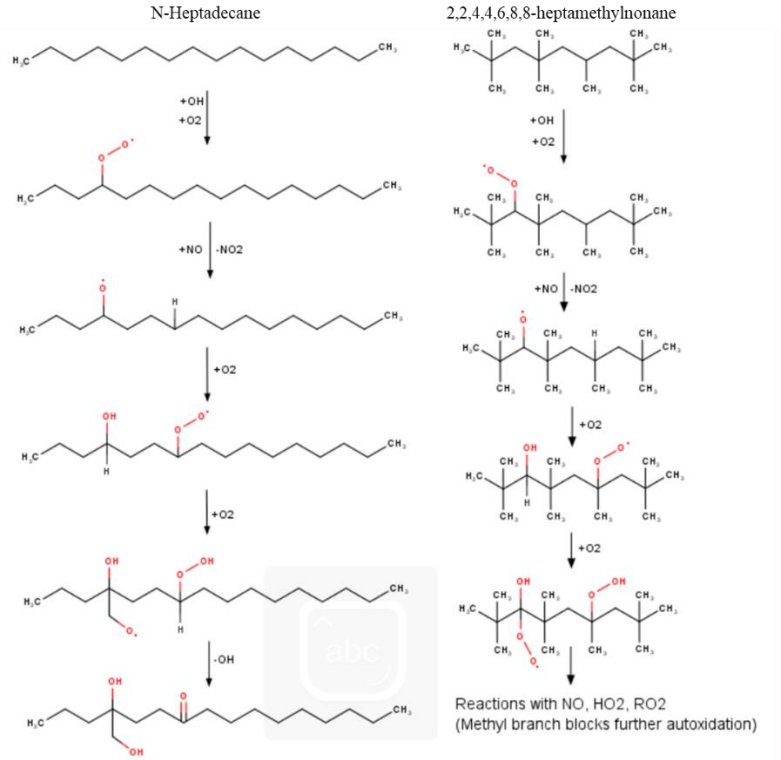
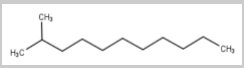
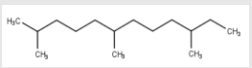
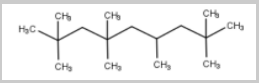
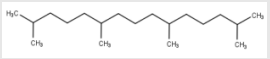


Figure S1. Comparison of autoxidation between linear Heptadecane (left) and 2,2,4,4,6,8,8-Heptamethylnonane.

Section S2. Parameters used to generate lumping arrays and hydroxyl radical rate constants for branched alkanes used in chamber experiments

Table S1. Model parameters used to generate lumping arrays and hydroxyl radical rate constants for branched alkanes used in chamber experiments (Table 1)

Compound name	Autoxidation Reduction Factor	Linear alkane with Closest Vapor Pressure	Reaction Rate with Hydroxyl Radical (S^{-1})[a]	Structure
Isododecane	0.9375	C11	1.39 E-11	
2,6,10-trimethyldodecane	0.78	C13	1.87 E-11	
2,2,4,4,6,8,8-heptamethylnonane	0.08	C11	0.87 E-11	
2,6,10,14-tetramethylpentadecane	0.75	C17	2.42 E-11	

[a]Rate constants calculated using structure-reactivity relationship (Kwok and Atkinson, 1995)

Section S3. Physicochemical parameters of lumping species used for branched alkanes

Table S2. Molecular weight (MW), oxygen to carbon ratio (O:C), and Hydrogen bonding (HB) of the 48 lumping species used for branched alkane UNIPAR simulations.

Lumping Group	MW (g/mol)[a]	O:C[a, b]	HB[a]
1VF	239.63	0.500	0.67
2VF	218.87	0.500	0.67
3VF	198.12	0.500	0.67
4VF	177.36	0.500	0.67
5VF	156.60	0.333	0.67
6VF	135.84	0.648	0.681842
7VF	115.08	0.899	0.625856
8VF	94.33	0.676	0.67
1F	138.32	0.500	0.67
2F	131.67	0.500	0.67
3F	125.02	0.500	0.67
4F	118.37	0.563	0.5
5F	111.72	0.500	0.25
6F	105.07	0.703	0.75
7F	98.41	0.583	0.666667
8F	91.76	0.557	0.67
1M	126.63	0.333	0.67
2M	123.87	0.333	0.67
3M	121.10	0.333	0.67
4M	118.34	0.750	1.25
5M	115.57	0.775	1.999998
6M	112.81	0.857	0.75
7M	110.04	0.424	0.966034
8M	107.28	0.270	0.136486
1S[c]	113.65+10.15*n	0.421	1.353102
2S	214.89	0.432	1.65
3S	203.01	0.434	0.774273
4S	191.13	0.436	1.273461
5S	179.25	0.180	0.999851
6S	167.37	0.533	0.4716
7S	155.49	0.301	0.496453
8S	143.61	0.548	0.061368
1P[c]	105.17+14.5*n	0.498	1.500002
2P	218.63	0.630	1.650003
3P	207.09	0.761	0.937543
4P	195.55	0.360	0.62506
5P	184.01	0.521	0.743975

6P	172.46	0.581	0.41964
7P	160.92	0.562	0.315915
8P	149.38	1.772	0.239521
1MA	210.18	0.330	3
2MA	198.63	0.330	3
3MA	106.12	0.750	3
4MA	120.40	0.621	3
5MA	164.01	0.330	3
6MA	152.46	0.330	3
7MA	140.92	0.330	3
8MA	129.38	0.330	3

[a] The unified parameter arrays were calculated by Madhu et al. (2023) as an average of the respective arrays generated from lumping explicit species from mechanisms of linear alkanes C9 to C12. Any parameters for lumping groups not populated by chemical species were extrapolated from adjacent groups within the same reactivity scale. [b] This table displays the base unified O:C array. Before application to the branched alkane UNIPAR model, an O:C reduction factor was applied to this array according to Eq. S1 below. [c] MW values for groups 1S and 1P were calculated as a function of their carbon number (n). Further description can be found below.

Table S2. displays the physicochemical parameters associated with the alkane UNIPAR model. These parameters were generated in the unification process described by Madhu et al. (2023). Within the molecular weight (MW) array, lumping groups 1P and 1S are incremented according to carbon number (n). This incrementation is fit to the incrementation of the respective 1P and 1S lumped arrays of explicitly predicted products of the mechanisms of linear alkanes C9-C12. The MWs of all volatility groups with higher vapor pressures (VP) values than group 1 are static. This is due to the assumption that, as MW increases, volatility will decrease as well, causing the higher MW species to automatically shift down to lower volatility groups. Thus, all but the lowest volatility group should have roughly the same MW value as the carbon number of the precursor increases. Groups 1VF, 1F, 1M, and 1MA were not incremented in this way as they were not sufficiently populated to fit.

As carbon number increases of an alkane precursor increases, oxygen-to-carbon ratio (O:C) values of the respective products, and thus lumping arrays, will also decrease. To account for this, an O:C reduction factor was applied to branched alkane O:C arrays which was calculated as follows:

$$O{:}C\ reduction\ factor = 10.5/n \qquad \text{(Eq. S1)}$$

which was applied by multiplying the O:C array displayed in table S2 by multiplying by this factor for each respective branched alkane. The numerator, 10.5, was chosen as the representative carbon number of the base O:C array as it is an average generated from the mechanisms of linear C9-C12.

Section S4. Lumping arrays for each branched alkane used for chamber simulations

Table S3. α-values used for the respective lumping arrays of Isododecane, 2,6,10-trimethyldodecane, 2,2,4,4,6,8,8-heptamethylnonane, and 2,6,10,14-tetramethylpentadecane under fresh high NO_x, fresh low NO_x, aged high NO_x, aged low NO_x.

Isododecane Fresh								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

6M	-4.06E-09	3.33E-07	-5.93E-06	3.10E-04	-6.46E-07	1.01E-05	-5.39E-05	3.89E-04
7M	-1.70E-08	1.38E-06	-2.34E-05	1.36E-03	-2.78E-06	4.29E-05	-2.25E-04	1.69E-03
8M	-1.55E-08	1.26E-06	-2.10E-05	1.26E-03	-2.55E-06	3.94E-05	-2.05E-04	1.56E-03
1S	-6.62E-09	1.37E-06	-1.27E-06	8.97E-05	1.60E-08	3.00E-07	9.92E-06	5.59E-05
2S	-6.98E-08	1.37E-05	4.45E-05	1.06E-03	5.16E-07	-4.30E-06	2.04E-04	6.19E-04
3S	9.11E-08	-6.80E-06	7.84E-04	3.36E-02	-1.89E-05	2.55E-04	-1.26E-04	3.38E-02
4S	7.19E-07	-8.10E-05	2.68E-03	1.47E-01	-9.27E-05	1.27E-03	-2.67E-03	1.51E-01
5S	6.73E-07	-7.42E-05	2.27E-03	1.38E-01	-9.03E-05	1.25E-03	-3.07E-03	1.42E-01
6S	-4.72E-08	3.38E-06	-1.48E-05	5.06E-03	-1.12E-05	1.68E-04	-7.82E-04	6.17E-03
7S	-5.65E-08	4.11E-06	-1.79E-05	5.95E-03	-1.30E-05	1.97E-04	-9.09E-04	7.23E-03
8S	-1.45E-08	1.10E-06	-3.70E-06	1.44E-03	-3.19E-06	4.81E-05	-2.20E-04	1.75E-03
1P	-1.18E-08	-7.41E-07	2.35E-04	6.10E-04	1.48E-06	-3.05E-05	4.26E-04	2.11E-04
2P	1.17E-08	-5.86E-06	6.54E-04	9.19E-03	-1.79E-06	2.44E-06	7.81E-04	8.52E-03
3P	1.74E-07	-1.91E-05	5.83E-04	3.56E-02	-2.33E-05	3.22E-04	-7.92E-04	3.67E-02
4P	1.62E-07	-1.78E-05	5.43E-04	3.33E-02	-2.18E-05	3.02E-04	-7.45E-04	3.43E-02
5P	1.27E-07	-1.41E-05	5.76E-04	3.06E-02	-1.99E-05	2.74E-04	-5.59E-04	3.14E-02
6P	5.89E-07	-6.54E-05	2.66E-03	1.39E-01	-9.16E-05	1.26E-03	-2.61E-03	1.43E-01
7P	5.75E-07	-6.35E-05	2.57E-03	1.30E-01	-8.94E-05	1.25E-03	-2.76E-03	1.34E-01
8P	2.91E-08	-2.88E-06	1.01E-04	-5.32E-05	-4.55E-06	8.16E-05	-3.85E-04	7.96E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (continued)

Isododecane Aged								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	-2.91E-09	2.56E-07	-7.47E-06	3.48E-04	-9.63E-07	1.75E-05	-1.13E-04	5.70E-04
6M	-4.73E-08	4.47E-06	-1.61E-04	6.27E-03	-1.04E-05	2.00E-04	-1.44E-03	9.18E-03
7M	-7.99E-08	7.59E-06	-2.78E-04	1.07E-02	-1.67E-05	3.25E-04	-2.38E-03	1.55E-02
8M	-3.41E-08	3.25E-06	-1.20E-04	4.57E-03	-7.00E-06	1.37E-04	-1.01E-03	6.61E-03

1S	-3.02E-07	2.03E-05	6.24E-04	-1.20E-03	-5.40E-06	1.47E-04	-5.27E-04	2.35E-03
2S	-1.20E-06	7.27E-05	3.52E-03	-4.27E-03	-2.56E-05	6.58E-04	-1.64E-03	1.14E-02
3S	-5.39E-08	2.12E-06	4.55E-04	9.87E-02	4.59E-05	-7.85E-04	4.89E-03	9.05E-02
4S	2.56E-07	-1.18E-06	-2.62E-03	1.82E-01	1.02E-04	-1.81E-03	8.38E-03	1.59E-01
5S	-2.18E-07	3.07E-05	-2.13E-03	1.02E-01	3.82E-06	3.99E-05	-2.86E-03	1.05E-01
6S	-5.88E-07	5.42E-05	-1.62E-03	5.01E-02	-9.39E-05	1.88E-03	-1.41E-02	7.95E-02
7S	-4.20E-07	3.84E-05	-1.04E-03	3.37E-02	-6.70E-05	1.34E-03	-9.82E-03	5.43E-02
8S	-9.34E-08	8.44E-06	-1.88E-04	6.77E-03	-1.49E-05	2.94E-04	-2.10E-03	1.12E-02
1P	4.74E-07	-4.81E-05	1.44E-03	2.69E-03	5.10E-07	-9.45E-05	2.18E-03	-1.88E-04
2P	5.67E-07	-5.44E-05	1.28E-03	2.78E-02	1.29E-05	-3.24E-04	3.42E-03	2.19E-02
3P	1.01E-08	4.94E-06	-8.00E-04	4.56E-02	2.23E-05	-3.86E-04	1.51E-03	4.09E-02
4P	4.41E-09	2.18E-06	-3.53E-04	2.02E-02	9.35E-06	-1.62E-04	6.17E-04	1.83E-02
5P	-1.77E-07	1.56E-05	-3.42E-04	1.06E-01	1.34E-05	-1.46E-04	-8.20E-05	1.07E-01
6P	-3.27E-07	2.87E-05	-6.15E-04	1.96E-01	2.39E-05	-2.55E-04	-2.22E-04	1.98E-01
7P	-1.45E-07	1.25E-05	-2.51E-04	8.64E-02	8.67E-06	-7.96E-05	-2.76E-04	8.80E-02
8P	-5.49E-10	-7.87E-08	1.08E-05	2.81E-04	-1.07E-06	1.88E-05	-1.04E-04	5.19E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.00E-06	1.00E-04	9.00E-04	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (continued)

2,6,10-Trimethyldodecane Fresh								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	-3.94E-09	3.80E-07	-7.79E-06	5.09E-04	-6.34E-07	1.16E-05	-7.29E-05	6.34E-04
7M	-1.01E-08	9.66E-07	-1.93E-05	1.33E-03	-1.64E-06	3.00E-05	-1.86E-04	1.65E-03
8M	-7.64E-09	7.31E-07	-1.44E-05	1.02E-03	-1.25E-06	2.29E-05	-1.41E-04	1.26E-03

1S	-6.72E-09	1.64E-06	4.86E-06	3.15E-04	-1.85E-08	7.83E-07	2.05E-05	2.51E-04
2S	-1.76E-08	6.01E-06	1.64E-04	8.31E-03	-2.42E-06	4.04E-05	7.63E-05	8.05E-03
3S	1.32E-07	-1.57E-05	9.27E-04	5.49E-02	-2.01E-05	3.24E-04	-5.93E-04	5.57E-02
4S	4.28E-07	-5.65E-05	2.15E-03	1.44E-01	-5.56E-05	9.03E-04	-2.36E-03	1.48E-01
5S	3.25E-07	-4.26E-05	1.55E-03	1.13E-01	-4.57E-05	7.49E-04	-2.23E-03	1.16E-01
6S	-2.94E-08	2.50E-06	-1.29E-05	5.19E-03	-6.92E-06	1.23E-04	-6.76E-04	6.33E-03
7S	-2.93E-08	2.53E-06	-1.29E-05	5.08E-03	-6.75E-06	1.20E-04	-6.57E-04	6.18E-03
8S	-7.12E-09	6.41E-07	-2.54E-06	1.17E-03	-1.57E-06	2.79E-05	-1.51E-04	1.42E-03
1P	-4.50E-09	-8.87E-07	2.13E-04	1.53E-03	5.40E-07	-1.60E-05	3.46E-04	1.16E-03
2P	2.93E-08	-6.25E-06	5.25E-04	1.50E-02	-4.01E-06	5.38E-05	3.41E-04	1.47E-02
3P	1.04E-07	-1.35E-05	4.87E-04	3.52E-02	-1.39E-05	2.28E-04	-6.61E-04	3.62E-02
4P	9.66E-08	-1.26E-05	4.81E-04	3.38E-02	-1.34E-05	2.19E-04	-6.16E-04	3.47E-02
5P	1.30E-07	-1.71E-05	8.20E-04	5.11E-02	-2.03E-05	3.31E-04	-8.03E-04	5.24E-02
6P	3.52E-07	-4.61E-05	2.21E-03	1.36E-01	-5.48E-05	8.96E-04	-2.21E-03	1.40E-01
7P	2.86E-07	-3.72E-05	1.78E-03	1.05E-01	-4.44E-05	7.36E-04	-1.95E-03	1.09E-01
8P	1.43E-08	-1.67E-06	6.94E-05	-4.32E-05	-2.24E-06	4.74E-05	-2.64E-04	6.46E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (continued)

2,6,10-Trimethyldodecane Aged								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-4.24E-09	4.68E-07	-1.92E-05	9.10E-04	-1.02E-06	2.29E-05	-1.90E-04	1.36E-03
5M	-1.96E-08	2.18E-06	-9.29E-05	4.28E-03	-4.32E-06	9.84E-05	-8.38E-04	6.28E-03
6M	-3.67E-08	4.11E-06	-1.77E-04	8.08E-03	-7.78E-06	1.79E-04	-1.54E-03	1.17E-02
7M	-3.00E-08	3.37E-06	-1.46E-04	6.62E-03	-6.22E-06	1.43E-04	-1.24E-03	9.59E-03
8M	-8.78E-09	9.88E-07	-4.30E-05	1.94E-03	-1.80E-06	4.16E-05	-3.62E-04	2.81E-03

1S	-3.60E-07	2.71E-05	1.27E-03	3.66E-03	-5.36E-06	1.85E-04	-5.34E-04	1.05E-02
2S	-4.30E-07	3.28E-05	1.52E-03	7.00E-02	1.30E-05	-1.76E-04	2.07E-03	7.20E-02
3S	3.32E-08	4.55E-06	-1.22E-03	1.37E-01	4.06E-05	-8.34E-04	4.60E-03	1.23E-01
4S	-4.43E-08	1.52E-05	-1.96E-03	1.30E-01	2.05E-05	-3.76E-04	4.45E-04	1.25E-01
5S	-2.49E-07	3.03E-05	-1.49E-03	7.03E-02	-2.98E-05	7.40E-04	-7.45E-03	8.75E-02
6S	-2.74E-07	2.97E-05	-9.99E-04	3.75E-02	-4.37E-05	1.03E-03	-9.05E-03	5.99E-02
7S	-1.34E-07	1.44E-05	-4.44E-04	1.74E-02	-2.13E-05	5.02E-04	-4.34E-03	2.82E-02
8S	-2.40E-08	2.57E-06	-6.74E-05	2.88E-03	-3.83E-06	8.95E-05	-7.56E-04	4.77E-03
1P	3.28E-07	-3.84E-05	1.23E-03	1.36E-02	3.51E-06	-1.42E-04	2.40E-03	9.25E-03
2P	1.98E-07	-1.97E-05	1.82E-04	4.46E-02	1.29E-05	-3.05E-04	2.44E-03	3.82E-02
3P	-8.99E-09	3.55E-06	-4.58E-04	4.12E-02	9.29E-06	-1.82E-04	7.73E-04	3.85E-02
4P	-7.15E-08	8.23E-06	-3.21E-04	8.03E-02	7.83E-06	-1.18E-04	1.68E-04	8.04E-02
5P	-1.46E-07	1.52E-05	-3.86E-04	1.45E-01	1.07E-05	-1.34E-04	-1.43E-04	1.47E-01
6P	-1.24E-07	1.28E-05	-3.17E-04	1.23E-01	8.47E-06	-1.02E-04	-1.97E-04	1.24E-01
7P	-3.74E-08	3.77E-06	-8.62E-05	3.68E-02	1.94E-06	-1.80E-05	-1.39E-04	3.76E-02
8P	-1.41E-10	-2.39E-08	3.87E-06	1.19E-04	-2.74E-07	5.72E-06	-3.73E-05	2.21E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.00E-06	1.00E-04	9.00E-04	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (continued)

2,2,4,4,6,8,8-Heptamethylnonane Fresh								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	-4.06E-09	3.33E-07	-5.93E-06	3.10E-04	-6.46E-07	1.01E-05	-5.39E-05	3.89E-04
7M	-1.70E-08	1.38E-06	-2.34E-05	1.36E-03	-2.78E-06	4.29E-05	-2.25E-04	1.69E-03
8M	-1.55E-08	1.26E-06	-2.10E-05	1.26E-03	-2.55E-06	3.94E-05	-2.05E-04	1.56E-03

1S	-1.85E-09	3.82E-07	-3.55E-07	2.50E-05	4.38E-09	8.51E-08	2.76E-06	1.56E-05
2S	-1.89E-08	3.84E-06	1.46E-06	2.66E-04	7.55E-08	2.15E-07	3.70E-05	1.62E-04
3S	1.44E-07	-1.44E-05	5.54E-04	3.25E-02	-2.05E-05	2.84E-04	-6.18E-04	3.32E-02
4S	7.30E-07	-8.03E-05	2.45E-03	1.47E-01	-9.41E-05	1.30E-03	-3.07E-03	1.51E-01
5S	6.73E-07	-7.42E-05	2.27E-03	1.38E-01	-9.03E-05	1.25E-03	-3.07E-03	1.42E-01
6S	-4.72E-08	3.38E-06	-1.48E-05	5.06E-03	-1.12E-05	1.68E-04	-7.82E-04	6.17E-03
7S	-5.65E-08	4.11E-06	-1.79E-05	5.95E-03	-1.30E-05	1.97E-04	-9.09E-04	7.23E-03
8S	-1.45E-08	1.10E-06	-3.70E-06	1.44E-03	-3.19E-06	4.81E-05	-2.20E-04	1.75E-03
1P	-1.04E-09	-6.52E-08	2.06E-05	5.36E-05	1.30E-07	-2.68E-06	3.75E-05	1.86E-05
2P	3.59E-08	-4.35E-06	1.74E-04	7.95E-03	-4.81E-06	6.47E-05	-8.96E-05	8.09E-03
3P	1.74E-07	-1.91E-05	5.83E-04	3.56E-02	-2.33E-05	3.22E-04	-7.92E-04	3.67E-02
4P	1.62E-07	-1.78E-05	5.43E-04	3.33E-02	-2.18E-05	3.02E-04	-7.45E-04	3.43E-02
5P	1.27E-07	-1.41E-05	5.76E-04	3.06E-02	-1.99E-05	2.74E-04	-5.59E-04	3.14E-02
6P	5.89E-07	-6.54E-05	2.66E-03	1.39E-01	-9.16E-05	1.26E-03	-2.61E-03	1.43E-01
7P	5.75E-07	-6.35E-05	2.57E-03	1.30E-01	-8.94E-05	1.25E-03	-2.76E-03	1.34E-01
8P	2.91E-08	-2.88E-06	1.01E-04	-5.32E-05	-4.55E-06	8.16E-05	-3.85E-04	7.96E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (continued)

2,2,4,4,6,8,8-Heptamethylnonane Aged								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	-2.91E-09	2.56E-07	-7.47E-06	3.48E-04	-9.63E-07	1.75E-05	-1.13E-04	5.70E-04
6M	-4.73E-08	4.47E-06	-1.61E-04	6.27E-03	-1.04E-05	2.00E-04	-1.44E-03	9.18E-03
7M	-7.99E-08	7.59E-06	-2.78E-04	1.07E-02	-1.67E-05	3.25E-04	-2.38E-03	1.55E-02

8M	-3.41E-08	3.25E-06	-1.20E-04	4.57E-03	-7.00E-06	1.37E-04	-1.01E-03	6.61E-03
1S	-8.36E-08	5.58E-06	1.72E-04	-3.35E-04	-1.49E-06	4.06E-05	-1.48E-04	6.56E-04
2S	-3.72E-07	2.42E-05	8.59E-04	-1.45E-03	-7.01E-06	1.88E-04	-6.21E-04	3.10E-03
3S	-5.24E-08	1.41E-05	-1.32E-03	9.78E-02	5.32E-05	-9.14E-04	4.09E-03	8.72E-02
4S	1.04E-07	1.43E-05	-3.09E-03	1.81E-01	1.02E-04	-1.79E-03	7.76E-03	1.59E-01
5S	-2.18E-07	3.07E-05	-2.13E-03	1.02E-01	3.82E-06	3.99E-05	-2.86E-03	1.05E-01
6S	-5.88E-07	5.42E-05	-1.62E-03	5.01E-02	-9.39E-05	1.88E-03	-1.41E-02	7.95E-02
7S	-4.20E-07	3.84E-05	-1.04E-03	3.37E-02	-6.70E-05	1.34E-03	-9.82E-03	5.43E-02
8S	-9.34E-08	8.44E-06	-1.88E-04	6.77E-03	-1.49E-05	2.94E-04	-2.10E-03	1.12E-02
1P	4.17E-08	-4.23E-06	1.27E-04	2.37E-04	4.40E-08	-8.30E-06	1.92E-04	-1.61E-05
2P	5.49E-08	-2.33E-06	-2.83E-04	2.49E-02	1.23E-05	-2.22E-04	1.06E-03	2.21E-02
3P	1.01E-08	4.94E-06	-8.00E-04	4.56E-02	2.23E-05	-3.86E-04	1.51E-03	4.09E-02
4P	4.41E-09	2.18E-06	-3.53E-04	2.02E-02	9.35E-06	-1.62E-04	6.17E-04	1.83E-02
5P	-1.77E-07	1.56E-05	-3.42E-04	1.06E-01	1.34E-05	-1.46E-04	-8.20E-05	1.07E-01
6P	-3.27E-07	2.87E-05	-6.15E-04	1.96E-01	2.39E-05	-2.55E-04	-2.22E-04	1.98E-01
7P	-1.45E-07	1.25E-05	-2.51E-04	8.64E-02	8.67E-06	-7.96E-05	-2.76E-04	8.80E-02
8P	-5.49E-10	-7.87E-08	1.08E-05	2.81E-04	-1.07E-06	1.88E-05	-1.04E-04	5.19E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.00E-06	1.00E-04	9.00E-04	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (continued)

2,6,10,14-Tetramethylpentadecane Fresh								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	-2.70E-10	3.84E-08	-1.19E-06	1.05E-04	-4.26E-08	1.15E-06	-1.07E-05	1.32E-04
6M	-1.41E-09	1.98E-07	-5.91E-06	5.69E-04	-2.27E-07	6.08E-06	-5.55E-05	7.09E-04
7M	-3.16E-09	4.43E-07	-1.29E-05	1.31E-03	-5.16E-07	1.38E-05	-1.25E-04	1.62E-03
8M	-2.26E-09	3.17E-07	-9.12E-06	9.47E-04	-3.72E-07	9.91E-06	-8.93E-05	1.17E-03

1S	-2.24E-09	8.38E-07	7.99E-06	6.74E-04	-4.19E-08	1.23E-06	1.49E-05	6.03E-04
2S	-1.68E-09	1.99E-06	1.55E-04	1.22E-02	-1.25E-06	3.02E-05	1.19E-05	1.21E-02
3S	4.96E-08	-8.83E-06	6.91E-04	6.14E-02	-7.28E-06	1.72E-04	-5.04E-04	6.25E-02
4S	1.34E-07	-2.59E-05	1.44E-03	1.42E-01	-1.76E-05	4.17E-04	-1.61E-03	1.45E-01
5S	9.57E-08	-1.84E-05	9.83E-04	1.05E-01	-1.37E-05	3.29E-04	-1.45E-03	1.08E-01
6S	-9.42E-09	1.17E-06	-8.80E-06	5.18E-03	-2.21E-06	5.76E-05	-4.61E-04	6.31E-03
7S	-8.87E-09	1.12E-06	-8.27E-06	4.79E-03	-2.04E-06	5.31E-05	-4.24E-04	5.82E-03
8S	-2.11E-09	2.78E-07	-1.61E-06	1.08E-03	-4.65E-07	1.21E-05	-9.55E-05	1.31E-03
1P	-9.63E-10	-5.21E-07	1.54E-04	2.10E-03	1.09E-07	-6.03E-06	2.35E-04	1.74E-03
2P	1.16E-08	-3.27E-06	3.62E-04	1.70E-02	-1.59E-06	3.28E-05	1.75E-04	1.68E-02
3P	3.31E-08	-6.29E-06	3.34E-04	3.51E-02	-4.45E-06	1.06E-04	-4.50E-04	3.61E-02
4P	3.19E-08	-6.07E-06	3.48E-04	3.52E-02	-4.47E-06	1.07E-04	-4.33E-04	3.62E-02
5P	4.69E-08	-8.99E-06	6.31E-04	5.74E-02	-7.31E-06	1.74E-04	-6.21E-04	5.89E-02
6P	1.11E-07	-2.13E-05	1.49E-03	1.34E-01	-1.73E-05	4.13E-04	-1.50E-03	1.38E-01
7P	8.50E-08	-1.62E-05	1.13E-03	9.76E-02	-1.32E-05	3.21E-04	-1.25E-03	1.01E-01
8P	4.24E-09	-7.23E-07	4.40E-05	-3.99E-05	-6.63E-07	2.05E-05	-1.67E-04	5.98E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S3. (Continued)

2,6,10,14-Tetramethylpentadecane Aged								
	Low NO_x				High NO_x			
Lumped Species	A[a]	B[a]	C[a]	D[a]	A[a]	B[a]	C[a]	D[a]
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-3.99E-10	6.42E-08	-3.85E-06	2.65E-04	-9.58E-08	3.15E-06	-3.82E-05	3.98E-04
3M	-1.74E-09	2.83E-07	-1.74E-05	1.18E-03	-3.96E-07	1.31E-05	-1.62E-04	1.74E-03
4M	-5.02E-09	8.19E-07	-5.10E-05	3.43E-03	-1.10E-06	3.67E-05	-4.58E-04	5.02E-03
5M	-8.90E-09	1.46E-06	-9.15E-05	6.11E-03	-1.90E-06	6.38E-05	-8.00E-04	8.90E-03
6M	-9.34E-09	1.53E-06	-9.68E-05	6.43E-03	-1.96E-06	6.59E-05	-8.31E-04	9.33E-03
7M	-5.25E-09	8.62E-07	-5.47E-05	3.62E-03	-1.09E-06	3.66E-05	-4.64E-04	5.24E-03
8M	-1.16E-09	1.90E-07	-1.21E-05	7.99E-04	-2.37E-07	8.01E-06	-1.02E-04	1.15E-03

1S	-1.56E-07	1.76E-05	1.07E-03	4.05E-02	9.89E-07	1.86E-05	3.94E-04	4.64E-02
2S	-8.89E-08	1.26E-05	1.40E-05	1.35E-01	9.97E-06	-2.66E-04	2.40E-03	1.29E-01
3S	-1.49E-08	6.23E-06	-1.07E-03	1.22E-01	6.58E-06	-1.79E-04	6.00E-04	1.17E-01
4S	-5.22E-08	1.10E-05	-1.09E-03	8.98E-02	-3.23E-06	1.40E-04	-2.90E-03	9.82E-02
5S	-7.61E-08	1.27E-05	-7.59E-04	4.78E-02	-1.08E-05	3.80E-04	-5.14E-03	6.59E-02
6S	-5.61E-08	8.88E-06	-4.23E-04	2.35E-02	-8.95E-06	3.08E-04	-3.93E-03	3.78E-02
7S	-2.14E-08	3.38E-06	-1.49E-04	8.61E-03	-3.42E-06	1.17E-04	-1.48E-03	1.40E-02
8S	-3.17E-09	4.94E-07	-1.90E-05	1.18E-03	-5.05E-07	1.72E-05	-2.13E-04	1.96E-03
1P	1.21E-07	-2.00E-05	8.10E-04	3.29E-02	2.78E-06	-1.20E-04	2.18E-03	2.63E-02
2P	3.48E-08	-4.34E-06	-1.23E-04	6.54E-02	4.67E-06	-1.46E-04	1.37E-03	6.00E-02
3P	-1.81E-08	3.42E-06	-2.66E-04	7.36E-02	2.84E-06	-6.91E-05	2.56E-04	7.29E-02
4P	-3.48E-08	5.44E-06	-2.34E-04	1.12E-01	2.87E-06	-5.63E-05	-1.22E-05	1.13E-01
5P	-3.80E-08	5.73E-06	-2.10E-04	1.17E-01	2.65E-06	-4.74E-05	-1.11E-04	1.19E-01
6P	-2.19E-08	3.28E-06	-1.16E-04	6.74E-02	1.40E-06	-2.34E-05	-9.99E-05	6.85E-02
7P	-5.13E-09	7.48E-07	-2.41E-05	1.58E-02	2.29E-07	-2.51E-06	-5.10E-05	1.62E-02
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.00E-06	1.00E-04	9.00E-04	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

[a] The stoichiometric coefficient value is calculated by $\alpha = A * (\mathrm{HC/NO_x})^3 + B * (\mathrm{HC}/NOx)^2 + C * (\mathrm{HC}/NOx) + D$, where HC/NOx is defined as: ppb Carbon / NO_x ppb

Section S5. Gas simulations of chamber experiments (Table 1) by using the CB6 Ozone model

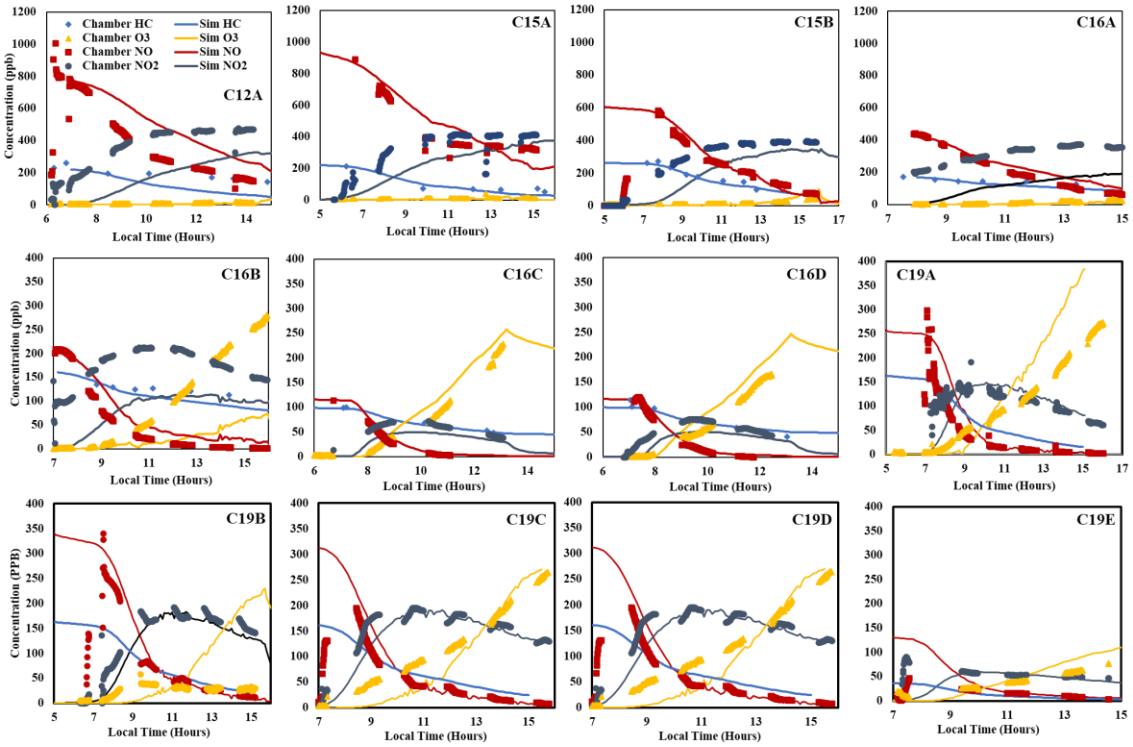


Figure S2. Chamber measurements and simulated concentrations of HC, Ozone, NO, and NO2 of experiments performed in this study reported in Table 1. Chamber measured concentrations of Tetramethylpentadecane (C19A-E) are not reported as this compound is too low volatility to be detected by the GC-FID appropriately; chamber simulations were performed with initial values of tetramethylpentadecane which were calculated according to the amount injected into the chamber assuming 95% injection efficiency.

Section S5. Sunlight profile used for sensitivity and uncertainty analyses

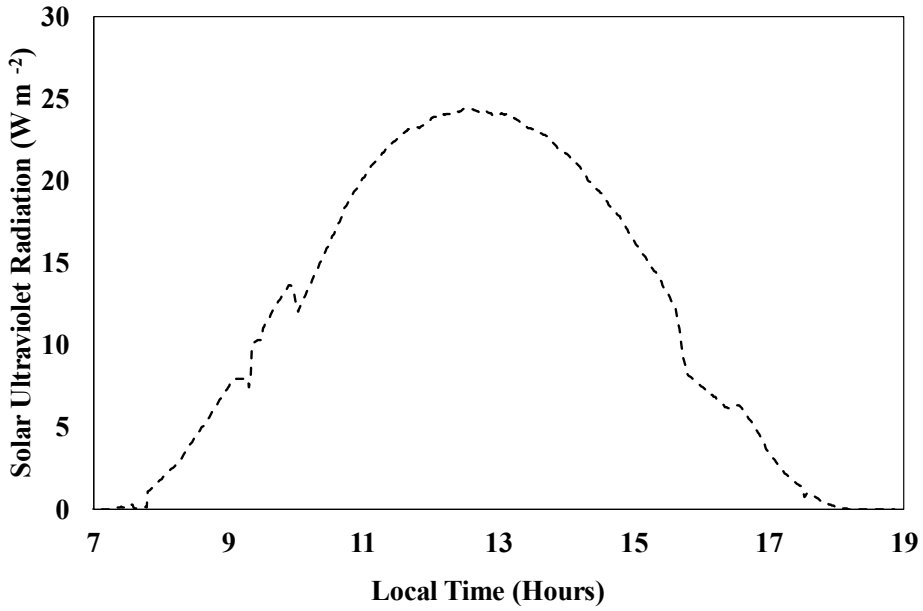
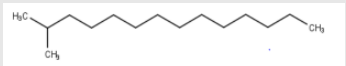
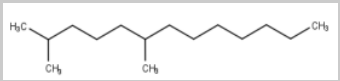
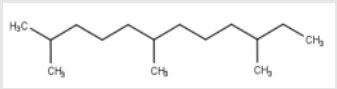
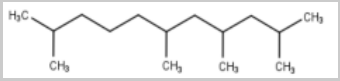


Figure S3. Time profile of reference sunlight radiance measure using Total Ultra-Violet Radiation (TUVR) in the UF-APHOR on 01/20/20. This sunlight profile is used for all sensitivity and uncertainty tests in this paper. This is the same sunlight profile used by Madhu et al. (2023) for sensitivity and uncertainty analysis.

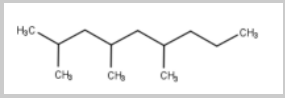
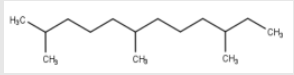
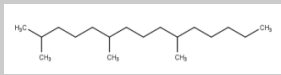
Section S4. Parameters used to generate lumping arrays and hydroxyl radical rate constants for branched alkanes used in sensitivity tests

Table S4. Parameters used to generate lumping arrays and hydroxyl radical rate constants for branched alkanes used in branching sensitivity test

Branching	Autoxidation Reduction Factor	Linear alkane with closest Vapor Pressure	Reaction Rate with Hydroxyl Radical (S^{-1})[a]	Structure
Linear	1	N/A	1.82 E-11	
1 Branch	0.98	C14	1.82 E-11	
2 Branch	0.84	C14	1.84 E-11	
3 Branch	0.78	C13	1.87 E-11	
4 Branch	0.72	C12	1.87 E-11	

[a]Rate constants calculated using structure-reactivity relationship (Kwok and Atkinson, 1995)

Table S5. Parameters used to generate lumping arrays and hydroxyl radical rate constants for branched alkanes used in NO_x and temperature sensitivity tests

Carbon Number	Autoxidation Reduction Factor	Linear alkane with Closest Vapor Pressure	Reaction Rate with Hydroxyl Radical (S^{-1})[a]	Structure
C12	0.84	C10	1.45 E-11	
C15	0.78	C13	1.87 E-11	
C18	0.72	C16	2.30 E-11	

[a]Rate constants calculated using structure-reactivity relationship (Kwok and Atkinson, 1995).

References

Kwok, E. S. C. and Atkinson, R.: Estimation of hydroxyl radical reaction rate constants for gas-phase organic compounds using a structure-reactivity relationship: An update, Atmospheric Environment, 29, 1685-1695, https://doi.org/10.1016/1352-2310(95)00069-B, 1995.

Madhu, A., Jang, M., and Deacon, D.: Modeling the influence of chain length on secondary organic aerosol (SOA) formation via multiphase reactions of alkanes, Atmos. Chem. Phys., 23, 1661-1675, 10.5194/acp-23-1661-2023, 2023.