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Modeling the influence of carbon branching structure on secondary organic aerosol formation via multiphase reactions of alkanes

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Section S1. CB6 Gas chemical mechanism

Simulations in this study were performed using the CB6r3 carbon bond mechanism (Emery et al., 2015). Within the mechanism, alkanes are input piecewise as "PAR", with 1 PAR representing 1 carbon on the precursor alkane structure. Using this chemical mechanism, the concentrations of RO_2, and HO_2 can be simulated for input to UNIPAR. Additionally, concentrations of NO, NO_2, and O_3 can be simulated for comparison to chamber data. Because the precursor alkanes are input piecewise, the concentrations of PAR cannot be used to input the simulated HC consumption to the UNIPAR model. To obtain simulated HC consumption from gas simulations, a reaction was added to the mechanism for each precursor HC as follows:

$$HC + OH = OH \qquad \text{(Eq. S1)}$$

Rate constants for the reaction of each precursor HC with OH were calculated using the framework outlined by Kwok and Atkinson (1995). With the inclusion of these reactions above, HC consumption was predicted while not impacting any underlying chemistry within the mechanism. The reaction rate of PAR groups with hydroxyl radicals in CB6 is based on a measured atmospheric set of alkanes which tend to much smaller that the precursors used in this study (Emery et al., 2015). Smaller alkanes tend to have a higher proportion of primary alkanes which decreases the per-carbon reactivity, relative to larger alkanes. Thus, the OH concentration used in Eq. S1 is likely too high as OH does not react quickly enough within the CB6 mechanism compared to chamber experiments with long-chain alkanes. Consequently, gas simulations have a slight tendency toward overprediction of hydrocarbon consumption simulated via Eq. S1.

Section S2. Basis for enthalpy of vaporization values

The enthalpy of vaporization (Chickos and Hanshaw, 2004) and vapor pressure (Myrdal and Yalkowsky, 1997; Zhao et al., 1999; Stein and Brown, 1994) values of a homologous series of alkanes were used to produce a regression equation to predict the enthalpy of vaporization at the vapor pressure for each given volatility group. As seen in Figure S1, enthalpy of vaporization values plateau after a sufficiently high vapor pressure. Thus, the three highest volatility bins are all assigned the same enthalpy of vaporization value.

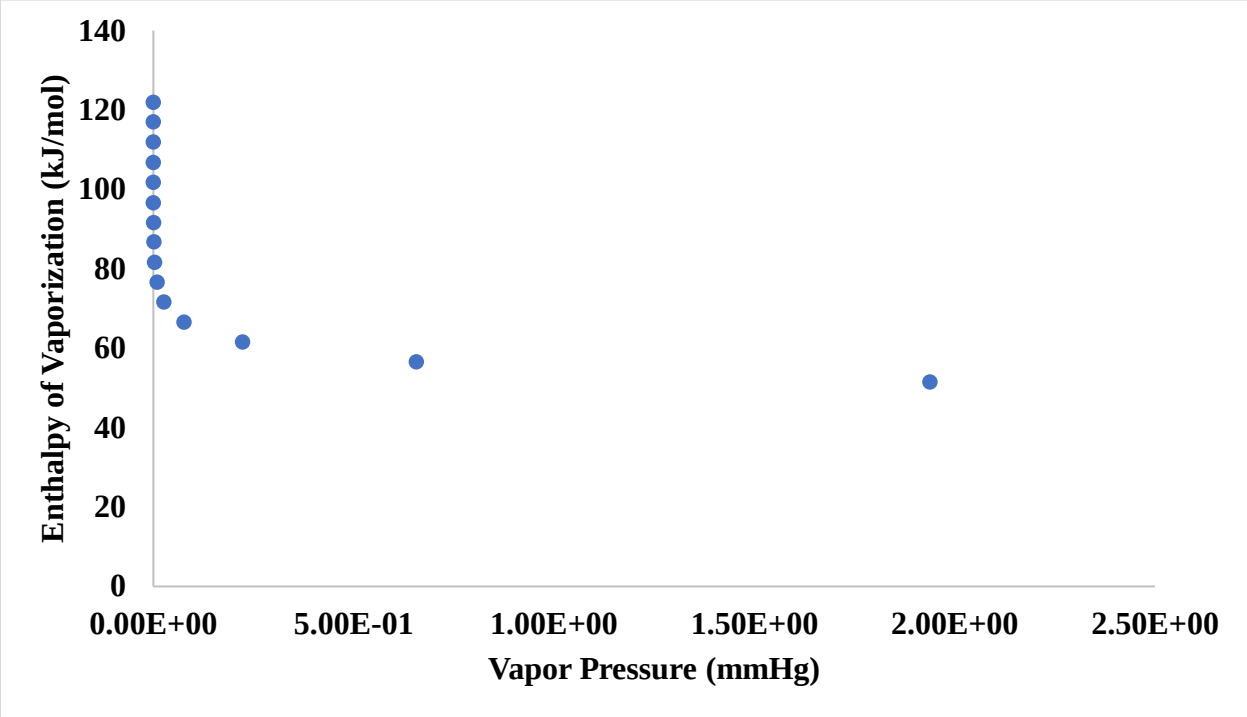


Figure S1. Enthalpy of Vaporization Vs. Vapor Pressure of n-Alkanes C9 to C24

Section S3. The basis for the calculation of the ARF

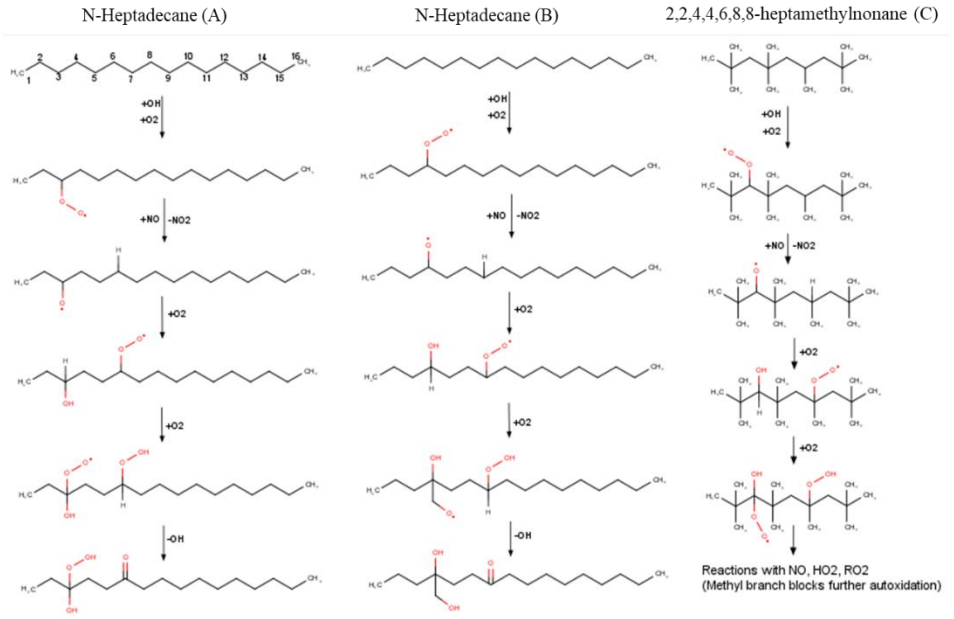


Figure S2. Comparison of autoxidation between linear heptadecane (left) and 2,2,4,4,6,8,8-heptamethylnonane. (A) autoxidation on carbons adjacent to the terminal carbons in heptadecane. (B) Autoxidation any secondary carbons in heptadecane except carbons adjacent to the terminal carbons. (C) autoxidation in 2,2,4,4,6,8,8-heptamethylnonane.

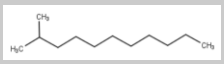
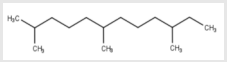
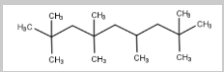
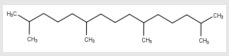
The basis for the calculation of the Autoxidation Reduction Factor (ARF) is as follows:

Generally, autoxidation is initiated by an alkoxy radical and proceeds via a 6-membered transition state (Praske et al., 2018; Atkinson, 2007). Terminal carbons are excluded from the ARF calculation due to a relatively weak reaction for OH hydrogen abstraction. Thus, the formation of an alkoxy radical from primary carbons is unlikely (Jenkin et al., 2018). Carbons on the alkane backbone in the α position relative to the terminal carbons are assigned an Autoxidation Potential (AP) value of 1 because autoxidation is only likely to occur on this carbon to one direction. Additionally, carbons on the alkane backbone in the β position relative to the terminal carbons are also assigned an AP value of 1 for the same reason (i.e. carbons 3 and 14 in Fig. S1A). For example, consider the case that a hydrogen atom is abstracted from carbon 2, 3, 14, or 15 in linear heptadecane in Fig. S1A. Following the reaction with NO, any of these alkoxy radicals can create a 6-membered transition state only in one direction (i.e. toward the center of the carbon backbone). Other carbons on the carbon backbone are assigned an AP value of 2 because autoxidation can occur in either direction due to the presence of hydrogens that are readily available for abstraction via a 6-membered transition state on either side of the chain. For example, the alkoxy radical present on carbon 4 in Fig. S1B can create a 6 membered transition state with a hydrogen attached to either carbon 1 or carbon 7 in linear heptadecane.

Another factor which will inhibit some autoxidation reactions is the presence of alkyl branches on the main carbon backbone. As seen in the n-heptadecane mechanisms Fig. S1A and Fig.S1B, if a hydrogen in a secondary carbon is oxidized with an OH radical and initiates autoxidation in the secondary carbon available to create a 6-membered transition state, this can produce highly oxidized molecule (HOM). However, as seen in the 2,2,4,4,6,8,8-heptamethylnonane mechanism (Fig. S1C), the presence of alkyl branches reduces hydrogen atoms that are available for abstraction via autoxidation. The carbon with one alkyl branch will be multiplied by a factor 0.5 as the number of hydrogens available for abstraction is decreased from two to one. Accordingly, the AP values for carbons on the main backbone with two alkyl branches are multiplied by a factor 0 as no hydrogens are available for abstraction.

Section S4. 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]	Reaction Rate with Hydroxyl Radical (S^{-1})[b]	Structure
Isododecane	0.821	C11	1.39 E-11	1.34 E-11	
2,6,10-trimethyldodecane	0.78	C13	1.87 E-11	1.78 E-11	
2,2,4,4,6,8,8-heptamethylnonane	0.36	C11	0.87 E-11	0.85 E-11	
2,6,10,14-tetramethylpentadecane	0.73	C17	2.42 E-11	2.31 E-11	

[a]Rate constants calculated using structure-reactivity relationship (Kwok and Atkinson, 1995)
[b]Rate constants calculated using structure-reactivity (Jenkin et al., 2018)

Rate constants calculated using the framework by Kwok and Atkinson (1995) were used for gas simulations in this study. For comparison, rate constants calculated by a more recent framework (Jenkin et al., 2018) are included and do not show significant differences.

Section S5. 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. S2 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:

$$O{:}C\ reduction\ factor = 10.5/n \qquad \text{(Eq. S2)}$$

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 S6. 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	-2.91E-09	2.56E-07	-7.47E-06	3.48E-04
6M	-4.06E-09	3.33E-07	-5.93E-06	3.10E-04	-4.73E-08	4.47E-06	-1.61E-04	6.27E-03
7M	-1.70E-08	1.38E-06	-2.34E-05	1.36E-03	-7.99E-08	7.59E-06	-2.78E-04	1.07E-02
8M	-1.55E-08	1.26E-06	-2.10E-05	1.26E-03	-3.41E-08	3.25E-06	-1.20E-04	4.57E-03
1S	-5.95E-09	1.23E-06	-1.14E-06	8.05E-05	-2.71E-07	1.82E-05	5.60E-04	-1.08E-03

2S	-6.25E-08	1.23E-05	3.84E-05	9.43E-04	-1.08E-06	6.58E-05	3.14E-03	-3.87E-03
3S	9.86E-08	-7.89E-06	7.52E-04	3.35E-02	-5.37E-08	3.83E-06	2.03E-04	9.86E-02
4S	7.21E-07	-8.09E-05	2.64E-03	1.47E-01	2.35E-07	1.02E-06	-2.69E-03	1.82E-01
5S	6.73E-07	-7.42E-05	2.27E-03	1.38E-01	-2.18E-07	3.07E-05	-2.13E-03	1.02E-01
6S	-4.72E-08	3.38E-06	-1.48E-05	5.06E-03	-5.88E-07	5.42E-05	-1.62E-03	5.01E-02
7S	-5.65E-08	4.11E-06	-1.79E-05	5.95E-03	-4.20E-07	3.84E-05	-1.04E-03	3.37E-02
8S	-1.45E-08	1.10E-06	-3.70E-06	1.44E-03	-9.34E-08	8.44E-06	-1.88E-04	6.77E-03
1P	-1.03E-08	-6.45E-07	2.04E-04	5.31E-04	4.13E-07	-4.19E-05	1.26E-03	2.34E-03
2P	1.51E-08	-5.65E-06	5.86E-04	9.01E-03	4.95E-07	-4.70E-05	1.06E-03	2.74E-02
3P	1.74E-07	-1.91E-05	5.83E-04	3.56E-02	1.01E-08	4.94E-06	-8.00E-04	4.56E-02
4P	1.62E-07	-1.78E-05	5.43E-04	3.33E-02	4.41E-09	2.18E-06	-3.53E-04	2.02E-02
5P	1.27E-07	-1.41E-05	5.76E-04	3.06E-02	-1.77E-07	1.56E-05	-3.42E-04	1.06E-01
6P	5.89E-07	-6.54E-05	2.66E-03	1.39E-01	-3.27E-07	2.87E-05	-6.15E-04	1.96E-01
7P	5.75E-07	-6.35E-05	2.57E-03	1.30E-01	-1.45E-07	1.25E-05	-2.51E-04	8.64E-02
8P	2.91E-08	-2.88E-06	1.01E-04	-5.32E-05	-5.49E-10	-7.87E-08	1.08E-05	2.81E-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	-3.99E-10	6.42E-08	-3.85E-06	2.65E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-1.74E-09	2.83E-07	-1.74E-05	1.18E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-5.02E-09	8.19E-07	-5.10E-05	3.43E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5M	-8.90E-09	1.46E-06	-9.15E-05	6.11E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	-9.34E-09	1.53E-06	-9.68E-05	6.43E-03	-6.46E-07	1.01E-05	-5.39E-05	3.89E-04
7M	-5.25E-09	8.62E-07	-5.47E-05	3.62E-03	-2.78E-06	4.29E-05	-2.25E-04	1.69E-03
8M	-1.16E-09	1.90E-07	-1.21E-05	7.99E-04	-2.55E-06	3.94E-05	-2.05E-04	1.56E-03
1S	-1.56E-07	1.76E-05	1.07E-03	4.05E-02	1.43E-08	2.70E-07	8.91E-06	5.02E-05
2S	-8.89E-08	1.26E-05	1.40E-05	1.35E-01	4.54E-07	-3.66E-06	1.80E-04	5.54E-04
3S	-1.49E-08	6.23E-06	-1.07E-03	1.22E-01	-1.91E-05	2.59E-04	-1.96E-04	3.37E-02

4S	-5.22E-08	1.10E-05	-1.09E-03	8.98E-02	-9.29E-05	1.27E-03	-2.73E-03	1.51E-01
5S	-7.61E-08	1.27E-05	-7.59E-04	4.78E-02	-9.03E-05	1.25E-03	-3.07E-03	1.42E-01
6S	-5.61E-08	8.88E-06	-4.23E-04	2.35E-02	-1.12E-05	1.68E-04	-7.82E-04	6.17E-03
7S	-2.14E-08	3.38E-06	-1.49E-04	8.61E-03	-1.30E-05	1.97E-04	-9.09E-04	7.23E-03
8S	-3.17E-09	4.94E-07	-1.90E-05	1.18E-03	-3.19E-06	4.81E-05	-2.20E-04	1.75E-03
1P	1.21E-07	-2.00E-05	8.10E-04	3.29E-02	1.29E-06	-2.65E-05	3.71E-04	1.84E-04
2P	3.48E-08	-4.34E-06	-1.23E-04	6.54E-02	-2.22E-06	1.13E-05	6.57E-04	8.46E-03
3P	-1.81E-08	3.42E-06	-2.66E-04	7.36E-02	-2.33E-05	3.22E-04	-7.92E-04	3.67E-02
4P	-3.48E-08	5.44E-06	-2.34E-04	1.12E-01	-2.18E-05	3.02E-04	-7.45E-04	3.43E-02
5P	-3.80E-08	5.73E-06	-2.10E-04	1.17E-01	-1.99E-05	2.74E-04	-5.59E-04	3.14E-02
6P	-2.19E-08	3.28E-06	-1.16E-04	6.74E-02	-9.16E-05	1.26E-03	-2.61E-03	1.43E-01
7P	-5.13E-09	7.48E-07	-2.41E-05	1.58E-02	-8.94E-05	1.25E-03	-2.76E-03	1.34E-01
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-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)

2,6,10-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	-6.70E-09	1.63E-06	4.85E-06	3.15E-04	-1.86E-08	7.84E-07	2.05E-05	2.51E-04
2S	-1.76E-08	5.99E-06	1.63E-04	8.31E-03	-2.42E-06	4.04E-05	7.58E-05	8.05E-03
3S	1.32E-07	-1.57E-05	9.27E-04	5.49E-02	-2.01E-05	3.24E-04	-5.94E-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	-4.48E-09	-8.85E-07	2.12E-04	1.53E-03	5.38E-07	-1.60E-05	3.45E-04	1.16E-03
2P	2.93E-08	-6.25E-06	5.24E-04	1.50E-02	-4.02E-06	5.39E-05	3.39E-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	-3.59E-07	2.71E-05	1.27E-03	3.66E-03	-5.35E-06	1.85E-04	-5.33E-04	1.05E-02
2S	-4.29E-07	3.28E-05	1.51E-03	7.00E-02	1.30E-05	-1.77E-04	2.07E-03	7.20E-02
3S	3.31E-08	4.57E-06	-1.22E-03	1.37E-01	4.06E-05	-8.34E-04	4.60E-03	1.23E-01
4S	-4.44E-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	3.27E-07	-3.83E-05	1.23E-03	1.36E-02	3.51E-06	-1.41E-04	2.40E-03	9.25E-03
2P	1.97E-07	-1.96E-05	1.79E-04	4.45E-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	-3.37E-09	6.97E-07	-6.47E-07	4.56E-05	8.07E-09	1.54E-07	5.04E-06	2.84E-05
2S	-3.51E-08	6.97E-06	1.52E-05	5.17E-04	2.16E-07	-1.22E-06	9.01E-05	3.08E-04
3S	1.27E-07	-1.20E-05	6.27E-04	3.28E-02	-2.00E-05	2.74E-04	-4.61E-04	3.34E-02
4S	7.27E-07	-8.05E-05	2.52E-03	1.47E-01	-9.37E-05	1.29E-03	-2.94E-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	-4.48E-09	-2.80E-07	8.89E-05	2.31E-04	5.61E-07	-1.15E-05	1.61E-04	7.99E-05
2P	2.82E-08	-4.83E-06	3.27E-04	8.34E-03	-3.85E-06	4.49E-05	1.88E-04	8.23E-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	-1.53E-07	1.03E-05	3.16E-04	-6.11E-04	-2.73E-06	7.44E-05	-2.69E-04	1.20E-03
2S	-6.35E-07	3.97E-05	1.71E-03	-2.35E-03	-1.29E-05	3.37E-04	-9.45E-04	5.73E-03

3S	-5.29E-08	1.03E-05	-7.56E-04	9.81E-02	5.09E-05	-8.73E-04	4.34E-03	8.82E-02
4S	1.52E-07	9.38E-06	-2.94E-03	1.81E-01	1.02E-04	-1.80E-03	7.96E-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	1.79E-07	-1.82E-05	5.46E-04	1.02E-03	1.92E-07	-3.58E-05	8.26E-04	-7.07E-05
2P	2.18E-07	-1.89E-05	2.14E-04	2.59E-02	1.25E-05	-2.54E-04	1.82E-03	2.20E-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	-5.48E-10	6.16E-08	-1.51E-06	1.05E-04	-8.67E-08	1.85E-06	-1.35E-05	1.32E-04
6M	-2.86E-09	3.18E-07	-7.49E-06	5.69E-04	-4.61E-07	9.76E-06	-7.04E-05	7.09E-04
7M	-6.42E-09	7.11E-07	-1.64E-05	1.31E-03	-1.05E-06	2.21E-05	-1.58E-04	1.62E-03
8M	-4.60E-09	5.08E-07	-1.16E-05	9.47E-04	-7.55E-07	1.59E-05	-1.13E-04	1.17E-03
1S	-4.45E-09	1.32E-06	9.99E-06	6.70E-04	-8.59E-08	1.99E-06	1.83E-05	6.01E-04
2S	-2.92E-09	3.07E-06	1.94E-04	1.22E-02	-2.55E-06	4.85E-05	1.07E-05	1.21E-02
3S	1.01E-07	-1.42E-05	8.72E-04	6.14E-02	-1.48E-05	2.76E-04	-6.46E-04	6.25E-02
4S	2.73E-07	-4.16E-05	1.82E-03	1.42E-01	-3.57E-05	6.70E-04	-2.05E-03	1.45E-01
5S	1.95E-07	-2.95E-05	1.25E-03	1.05E-01	-2.78E-05	5.28E-04	-1.83E-03	1.08E-01
6S	-1.91E-08	1.88E-06	-1.11E-05	5.18E-03	-4.49E-06	9.24E-05	-5.84E-04	6.31E-03
7S	-1.80E-08	1.79E-06	-1.05E-05	4.79E-03	-4.14E-06	8.51E-05	-5.37E-04	5.82E-03
8S	-4.29E-09	4.46E-07	-2.03E-06	1.08E-03	-9.45E-07	1.94E-05	-1.21E-04	1.31E-03
1P	-1.83E-09	-8.25E-07	1.90E-04	2.09E-03	2.05E-07	-9.24E-06	2.89E-04	1.73E-03
2P	2.38E-08	-5.22E-06	4.51E-04	1.69E-02	-3.25E-06	5.33E-05	2.09E-04	1.68E-02
3P	6.72E-08	-1.01E-05	4.23E-04	3.51E-02	-9.04E-06	1.71E-04	-5.70E-04	3.61E-02

4P	6.48E-08	-9.75E-06	4.41E-04	3.52E-02	-9.08E-06	1.71E-04	-5.48E-04	3.62E-02
5P	9.53E-08	-1.44E-05	8.00E-04	5.74E-02	-1.49E-05	2.80E-04	-7.86E-04	5.89E-02
6P	2.26E-07	-3.41E-05	1.89E-03	1.34E-01	-3.51E-05	6.63E-04	-1.90E-03	1.38E-01
7P	1.73E-07	-2.60E-05	1.43E-03	9.76E-02	-2.69E-05	5.14E-04	-1.58E-03	1.01E-01
8P	8.62E-09	-1.16E-06	5.57E-05	-3.99E-05	-1.35E-06	3.29E-05	-2.12E-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	-8.10E-10	1.03E-07	-4.88E-06	2.65E-04	-1.95E-07	5.05E-06	-4.84E-05	3.98E-04
3M	-3.54E-09	4.54E-07	-2.20E-05	1.18E-03	-8.06E-07	2.11E-05	-2.05E-04	1.74E-03
4M	-1.02E-08	1.31E-06	-6.46E-05	3.43E-03	-2.24E-06	5.90E-05	-5.80E-04	5.02E-03
5M	-1.81E-08	2.34E-06	-1.16E-04	6.11E-03	-3.87E-06	1.02E-04	-1.01E-03	8.90E-03
6M	-1.90E-08	2.46E-06	-1.23E-04	6.43E-03	-3.98E-06	1.06E-04	-1.05E-03	9.33E-03
7M	-1.07E-08	1.38E-06	-6.93E-05	3.62E-03	-2.21E-06	5.88E-05	-5.88E-04	5.24E-03
8M	-2.35E-09	3.05E-07	-1.53E-05	7.99E-04	-4.82E-07	1.29E-05	-1.29E-04	1.15E-03
1S	-3.11E-07	2.79E-05	1.32E-03	4.05E-02	2.15E-06	2.51E-05	5.10E-04	4.63E-02
2S	-1.78E-07	2.01E-05	-2.10E-05	1.35E-01	2.04E-05	-4.31E-04	3.03E-03	1.29E-01
3S	-3.08E-08	1.01E-05	-1.37E-03	1.22E-01	1.34E-05	-2.87E-04	7.54E-04	1.17E-01
4S	-1.06E-07	1.77E-05	-1.39E-03	8.98E-02	-6.56E-06	2.25E-04	-3.67E-03	9.82E-02

5S	-1.55E-07	2.04E-05	-9.62E-04	4.78E-02	-2.19E-05	6.09E-04	-6.51E-03	6.59E-02
6S	-1.14E-07	1.42E-05	-5.35E-04	2.35E-02	-1.82E-05	4.95E-04	-4.98E-03	3.78E-02
7S	-4.36E-08	5.42E-06	-1.88E-04	8.61E-03	-6.95E-06	1.88E-04	-1.87E-03	1.40E-02
8S	-6.44E-09	7.93E-07	-2.40E-05	1.18E-03	-1.03E-06	2.77E-05	-2.70E-04	1.96E-03
1P	2.39E-07	-3.12E-05	9.91E-04	3.28E-02	5.64E-06	-1.91E-04	2.70E-03	2.63E-02
2P	6.87E-08	-6.68E-06	-1.67E-04	6.54E-02	9.49E-06	-2.34E-04	1.71E-03	6.00E-02
3P	-3.68E-08	5.49E-06	-3.36E-04	7.36E-02	5.77E-06	-1.11E-04	3.24E-04	7.29E-02
4P	-7.08E-08	8.72E-06	-2.96E-04	1.12E-01	5.82E-06	-9.03E-05	-1.54E-05	1.13E-01
5P	-7.71E-08	9.20E-06	-2.65E-04	1.17E-01	5.39E-06	-7.61E-05	-1.40E-04	1.19E-01
6P	-4.44E-08	5.26E-06	-1.47E-04	6.74E-02	2.84E-06	-3.76E-05	-1.27E-04	6.85E-02
7P	-1.04E-08	1.20E-06	-3.05E-05	1.58E-02	4.65E-07	-4.03E-06	-6.47E-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 $\alpha = A * (\mathrm{HC}/\mathrm{NO_x})^3 + B * (\mathrm{HC}/NOx)^2 + C * (\mathrm{HC}/NOx) + D$, where HC(Hydrocarbon)/NOx is defined as: ppb Carbon / NO_x ppb

Parameters for high NO_x should be used when HC ppbC / NO_x ppb ≤ 5 and Parameters for low NO_x should be used when HC ppbC / NO_x ppb > 5.

Section S7. Gas simulations of chamber experiments (Table 1) by using the CB6 Ozone model

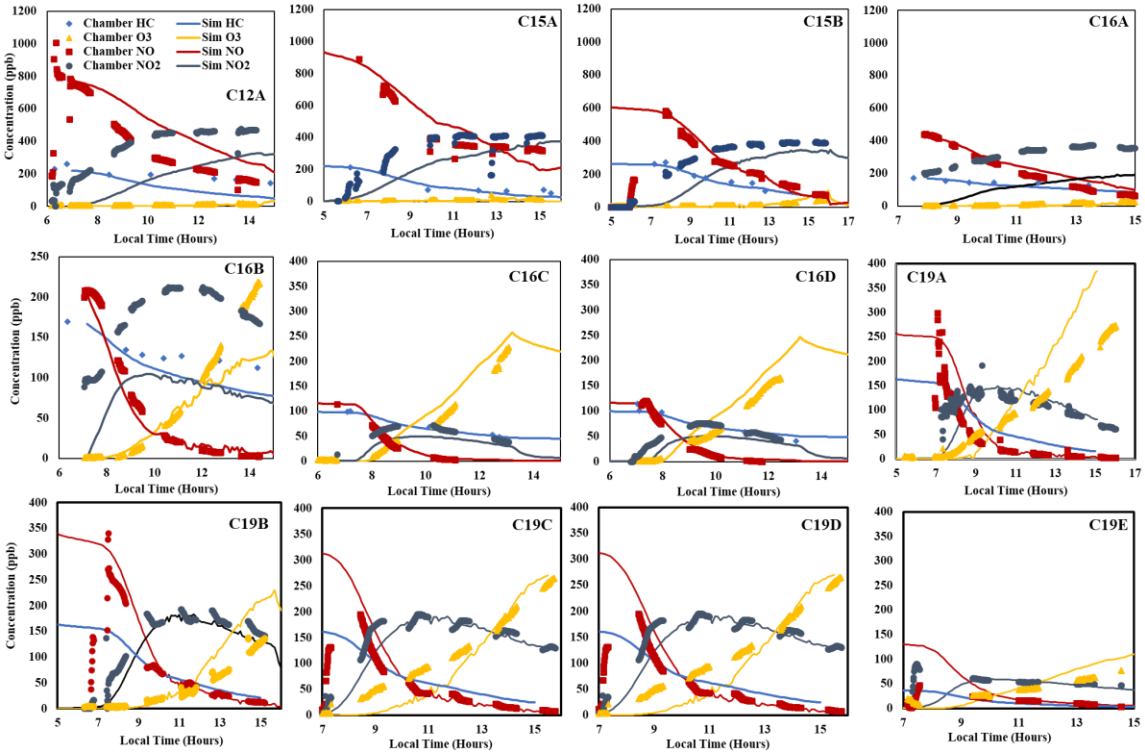


Figure S3. Chamber measurements and simulated concentrations of HC, Ozone, NO, and NO2 of experiments performed in this study reported in Table 1. Chamber measured concentrations of Tetramethylpentadecane (C19A-E) are not reported as this compound is too low volatility to be detected by the GC-FID appropriately; 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 S8. Description of FTIR analysis

FTIR spectra from numerous chemical species, varying in functional groups and carbon lengths, were collected from the NIST Quantitative Infrared Database (Chu et al., 1999) and measured from SOA related compounds (i.e. pinonaldehyde and pinoic acid). The collected spectra are used to identify peaks for specific functional groups in spectra obtained from SOA chamber experiments.

Table S4. Peak assignments of FTIR spectra

Functional group	Peak ranges cm^{-1}	O content	C content
OH stretching in alcohol	3650-3200	1	0
OH stretching in carboxylic acid	3550-2500	2	1
CH stretching	2861, 2927, 2972	0	1
C=O stretching in ketone and carboxylic acid	1725	1	1
C-O stretching (non-carboxylic acid and non-alcohols)	1080-1240	1	1

Table S4 reports peak ranges for various functional groups identified in Figure 4. To calculate O:C values, the sum of the areas of all peaks belonging to each functional group was converted to the relative intensity for each functional group. After being normalized by the CH stretching intensity, the relative intensities are used, alongside the values for oxygen content and carbon content, to calculate O:C values.

Section S9. Sunlight profile used for sensitivity and uncertainty analyses

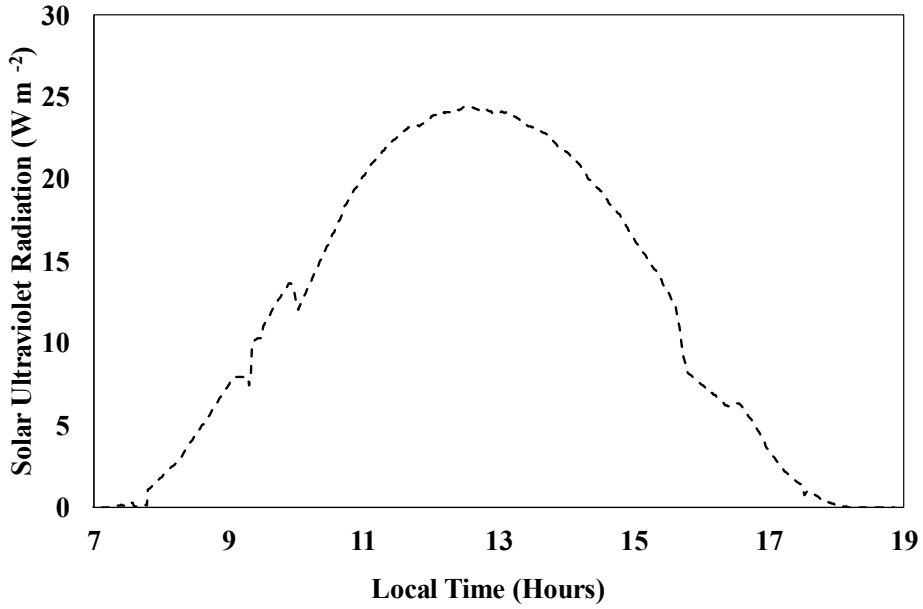
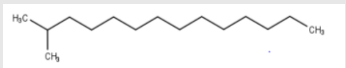
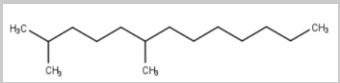
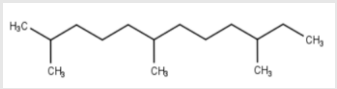
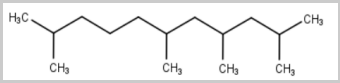


Figure S4. Time profile of reference sunlight radiance measure using Total Ultra-Violet Radiation (TUVR) in the UF-APHOR on 01/20/20. This sunlight profile is used for all sensitivity and uncertainty tests in this paper. This is the same sunlight profile used by Madhu et al. (2023) for sensitivity and uncertainty analysis.

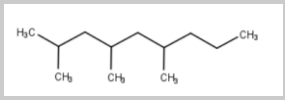
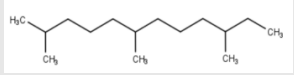
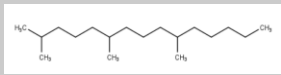
Section S10. Parameters used to generate lumping arrays and hydroxyl radical rate constants for branched alkanes used in sensitivity tests

Table S5. 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	0.83	C14	1.84 E-11	
3 Branch	0.78	C13	1.87 E-11	
4 Branch	0.69	C12	1.87 E-11	

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

Table S6. 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	0.67	C10	1.45 E-11	
C15	0.78	C13	1.87 E-11	
C18	0.81	C16	2.30 E-11	

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

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