



Supplement of

Secondary organic aerosol formation via multiphase reaction of hydrocarbons in urban atmospheres using CAMx integrated with the UNIPAR model

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Section S1: SOA prediction with the UNIPAR model

The mass-based stoichiometric coefficient (α_i) of each lumping species i can be calculated based the variables listed in Table S3. Both the stoichiometric coefficient array derived from the fresh compositions and that from the aged compositions are determined as a function of NO_x levels using the mathematical equations. To simulate age-dependent SOA formation, the stoichiometric coefficient array is reconstructed over time by a weighted average of fresh and aged stoichiometric coefficients based on the normalized concentration of oxidized organic radicals and HO_2 with a hydrocarbon concentration. The detailed information of the calculation of age-dependent stoichiometric coefficient of lumping species was discussed in the previous study (Zhou et al., 2019).

In UNIPAR model, SOA formation is estimated by both the partitioning process and aerosol-phase heterogeneous reactions. The detailed parameters of UNIPAR model has been described in previous studies (Im et al., 2014; Beardsley and Jang, 2016; Zhou et al., 2019; Han and Jang, 2020; Yu et al., 2021b). Briefly, the gaseous SOA products predicted by explicit gas mechanisms are distributed into both inorganic phase and organic phase through multiphase partitioning. The partitioning coefficient of each lumping species in inorganic phase ($K_{in,i}$, $\text{m}^3 \mu\text{g}^{-1}$) and in organic phase ($K_{or,i}$, $\text{m}^3 \mu\text{g}^{-1}$) are calculated as follows,

$$K_{in,i} = \frac{7.501 RT}{10^9 MW_{in} \gamma_{in,i} p_{l,i}^0}, \quad (\text{S1})$$

$$K_{or,i} = \frac{7.501 RT}{10^9 MW_{or} \gamma_{or,i} p_{l,i}^0} \quad (\text{S2})$$

where R is the ideal gas constant, T (K) is temperature, MW (g mol^{-1}) is the molecular weight of medium, γ is the activity coefficient of the species i in the medium, and p (mmHg) is the liquid vapor pressure of species i . The γ_{or} value is assumed to be unity. The γ_{in} value is estimated based on a semiempirically derived regression equation which is obtained by fitting the equation to Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficient (AIOMFAC)-predicted γ (Zuend et al., 2011) in the presence of organics, ammonium, sulfate, and nitrate as follows,

$$\gamma_{in,i} = e^{0.037 MW_i - 2.998 \ln(O:C_i) - 0.970 HB_i + 12.19 f_{anion} - 1.725 f_{nitrate} - 8.043 RH} \quad (\text{S3})$$

where RH is relative humidity (0-1), f_{anion} and $f_{nitrate}$ are the inorganic composition parameters and can be calculated as,

$$f_{anion} = \frac{n(NO_3^-) + 2 \times n(SO_4^{2-})}{n(NO_3^-) + 2 \times n(SO_4^{2-}) + n(NH_4^+)} \quad (S4)$$

and

$$f_{nitrate} = \frac{n(NO_3^-)}{n(NO_3^-) + n(SO_4^{2-})} \quad (S5)$$

The averaged molecular weight (MW), the hydrogen bonding parameter (HB), and the oxygen to carbon ratio ($O:C$) of the lumping species are shown in Table S4-S6, respectively.

For heterogeneous reactions, the kinetic equations for oligomerization in organic phase and salted aqueous phase were discussed in the previous studies (Zhou et al., 2019; Yu et al., 2021b; Han and Jang, 2021). The organic-phase reaction rate constant, $k_{o,i}$ ($L \text{ mol}^{-1} \text{ s}^{-1}$), and inorganic-phase rate constant, $k_{AC,i}$ ($L \text{ mol}^{-1} \text{ s}^{-1}$), are semiempirically derived by using various model compounds in the flow tube reactor (Jang et al., 2005). $k_{AC,i}$ is estimated as follows,

$$k_{AC,i} = 10^{0.95R_i + 0.25 pK_{BH^+}_i + 1.0 \cdot X + \log(a_w [H^+]) - 2.58} \quad (S6)$$

where R_i is the reactivity scale of the lumping species (Table S7), pK_{BH} is the basicity constant (Table S8), X is the excess acidity, a_w is the water activity and $[H^+]$ is concentration of protons.

For the highly reactive lumping species of VF, F, and M groups, $k_{o,i}$ are estimated as follows (Han and Jang, 2021),

$$k_{o,i} = 10^{0.95R_i + 0.25 pK_{BH^+}_i + 1.2 \times \left(1 - \frac{1}{1 + e^{0.005 \times (300 - MW_o)}}\right) + \frac{2.2}{1 + e^{6 \times (0.75 - O:C)}} - 6.3} + 1.1 \quad (S7)$$

For the lumping species of S, P and MA groups, $k_{o,i}$ are estimated as follows,

$$k_{o,i} = 10^{0.95R_i + 0.25 pK_{BH^+}_i + 1.2 \times \left(1 - \frac{1}{1 + e^{0.005 \times (300 - MW_o)}}\right) + \frac{2.2}{1 + e^{6 \times (0.75 - O:C)}} - 6.3} \quad (S8)$$

Table S1. Computation test for CAMx-UNIPAR and CAMx-SOAP for the KORUS-AQ case

Simulation index	Domain 1	Domain 2	MPI x OMP	1-Day simulation
CAMx	EA-27km	N/A	4x4	22.7 min
CAMx-UNIPAR	EA-27km	N/A	4x4	54.1 min
CAMx	EA-27km	SK-9km	6x4	36.3 min
CAMx-UNIPAR	EA-27km	SK-9km	6x4	74.6 min
CAMx	EA-27km	SK-9km	6x6	18.4 min
CAMx-UNIPAR	EA-27km	SK-9km	8x8	54.5 min

Section S2: Prediction of aerosol inorganic composition and aerosol acidity

Both the aerosol inorganic composition and aerosol acidity are estimated by using the ISORROPIA inorganic thermodynamic model (Nenes et al., 1998; Fountoukis and Nenes, 2007). In general, many thermodynamic models, such as E-AIM (Clegg et al., 1998) and ISORROPIA (Nenes et al., 1998; Fountoukis and Nenes, 2007), employ the ZSR relation to estimate water activity of the system that is directly related to the prediction of aerosol water content (Stokes and Robinson, 1966; Zdanovskii, 1948). It is known that the estimation of water prediction is relatively accurate and similar between models. However, the calculation of activity coefficient of the proton in the highly concentrated salted system are uncertain due to the lack of database and it is various between models as discussed in the previous studies (Jang et al., 2020; Pye et al., 2020). During the KORUS-AQ campaign, the inorganic acid was mostly titrated as shown in Figure S1-S3, and aerosol was near neutral. Thus, the aerosol water mass mainly influenced aqueous phase reactions of organics and their partitioning to aqueous phase.

In order to accurately predict the aerosol phase status (liquid or solid phase), the deliquescence relative humidity and the efflorescence relative humidity (ERH) are considered in the simulation of this study. The mutual deliquescence relative humidity (MDRH) is predicted by using ISORROPIA model. In a multicomponent inorganic mixture, the MDRH is the relative humidity that all salts are simultaneously saturated with respect to all components. The ERH (0-1) is predicted by using the neural network model based on inorganic composition (Yu et al., 2021a) and shown as following equations.

$$N_1 = 1.54463 \times f_{anion} - 0.9243 \times f_{nitrate} - 0.073745 \quad (S9)$$

$$N_2 = -0.63382 \times f_{anion} + 0.82856 \times f_{nitrate} + 0.288342 \quad (S10)$$

$$N_3 = -0.18594 \times f_{anion} + 0.63382 \times f_{nitrate} + 0.366726 \quad (S11)$$

$$N'_i = \begin{cases} N_i \geq 0, N_i \\ N_i < 0, 0 \end{cases} \quad i = 1,2,3 \quad (S12)$$

$$N_4 = -0.50581 \times N'_1 - 1.15781 \times N'_2 + 0.68805 \times N'_3 + 0.33499 \quad (S13)$$

$$N'_4 = \begin{cases} N_4 \geq 0, N_4 \\ N_4 < 0, 0 \end{cases} \quad (S14)$$

$$ERH = 2.21228 \times N'_4 + 0.00018 \quad (S15)$$

f_{anion} is calculated as the fraction of anion charges to total ion charges excluding proton and $f_{nitrate}$ is the mole fraction of nitrate to total anion.

Section S3: Measurements and predictions at four different observation sites

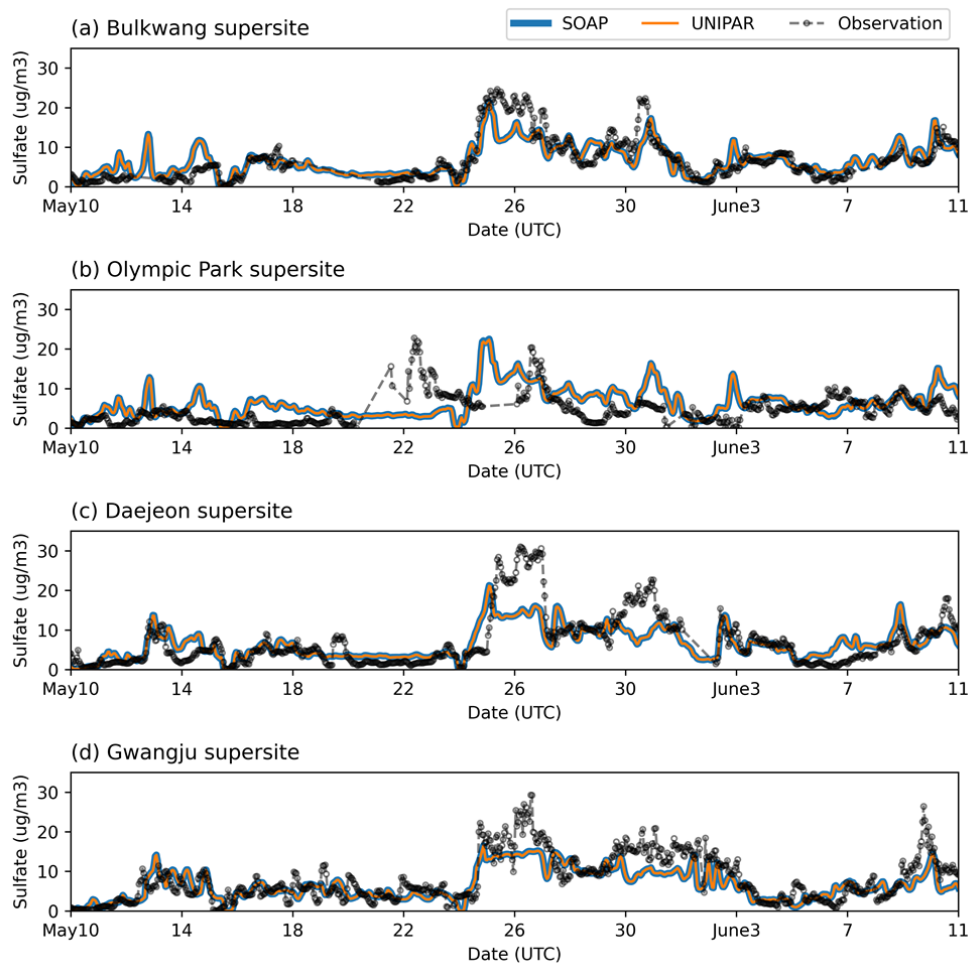


Figure S1. Time profiles of observed and predicted sulfate concentrations at (a) Bulkwang, (b) Olympic Park, (c) Daejeon, and (d) Gwangju supersites.

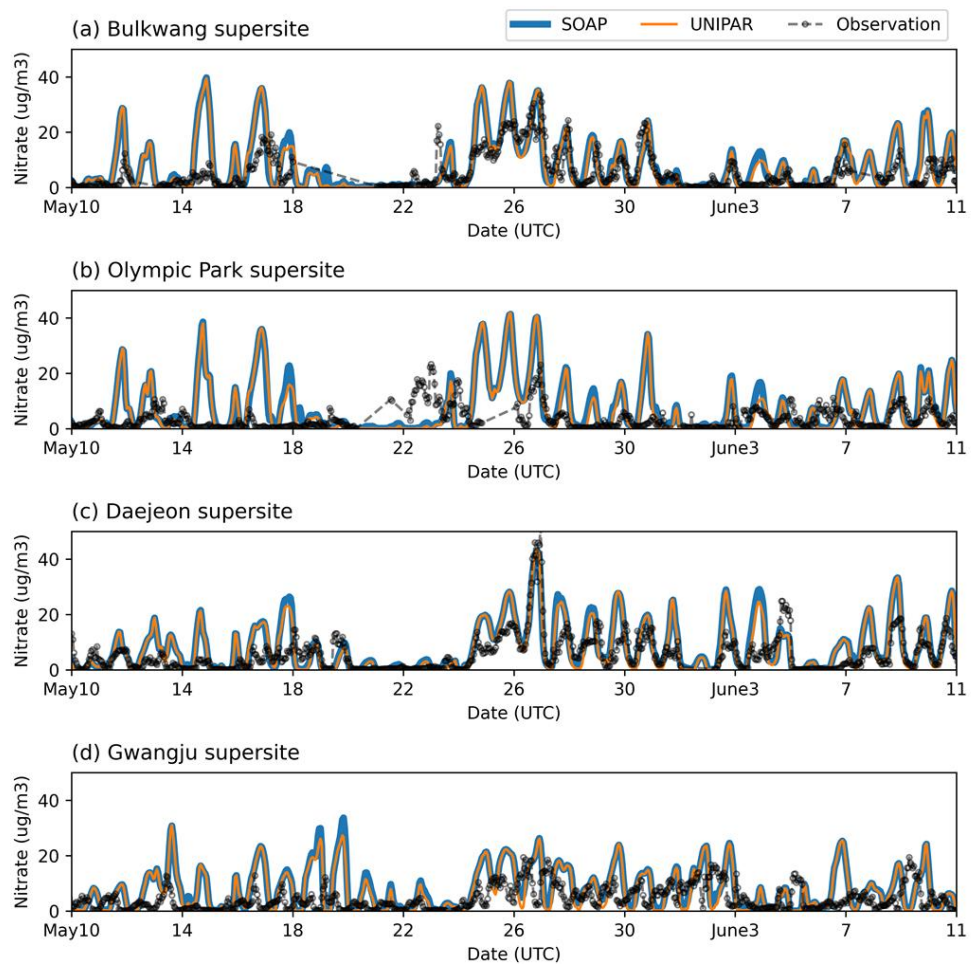


Figure S2. Time profiles of observed and predicted nitrate concentrations at (a) Bulkwang, (b) Olympic Park, (c) Daejeon, and (d) Gwangju supersites.

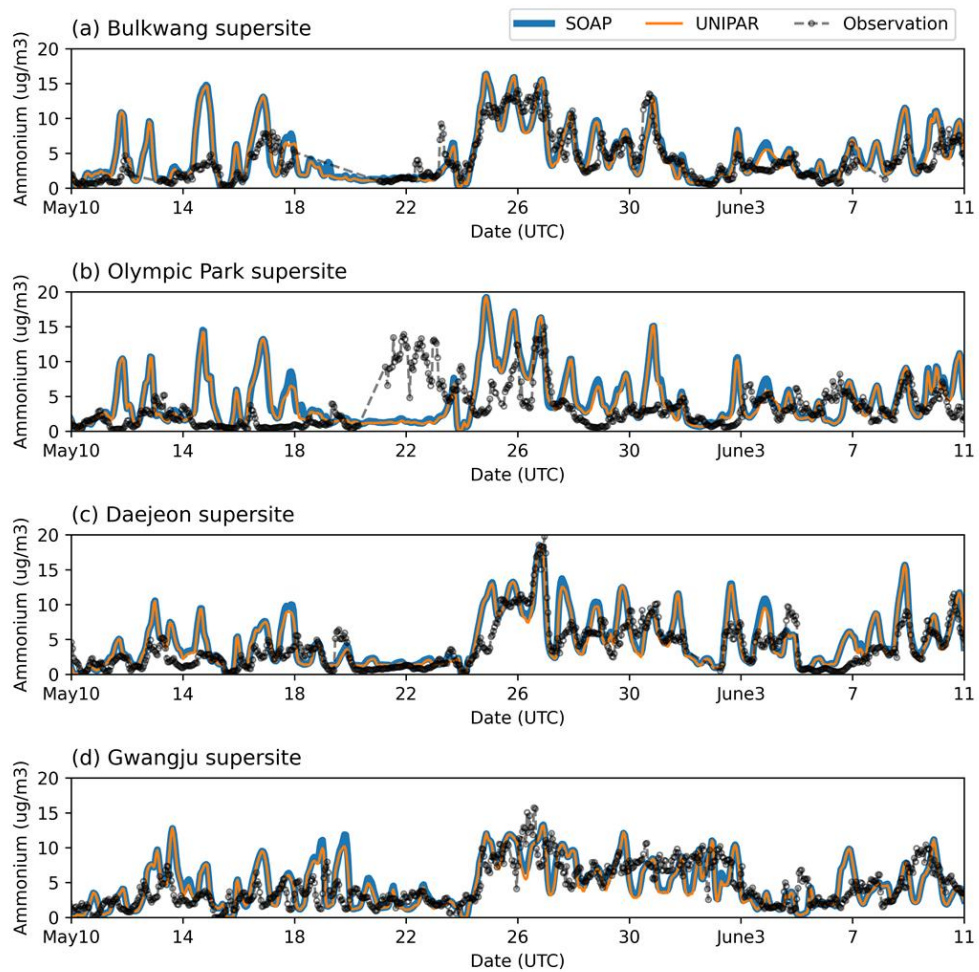


Figure S3. Time profiles of observed and predicted ammonium ion concentrations at (a) Bulkwang, (b) Olympic Park, (c) Daejeon, and (d) Gwangju supersites.

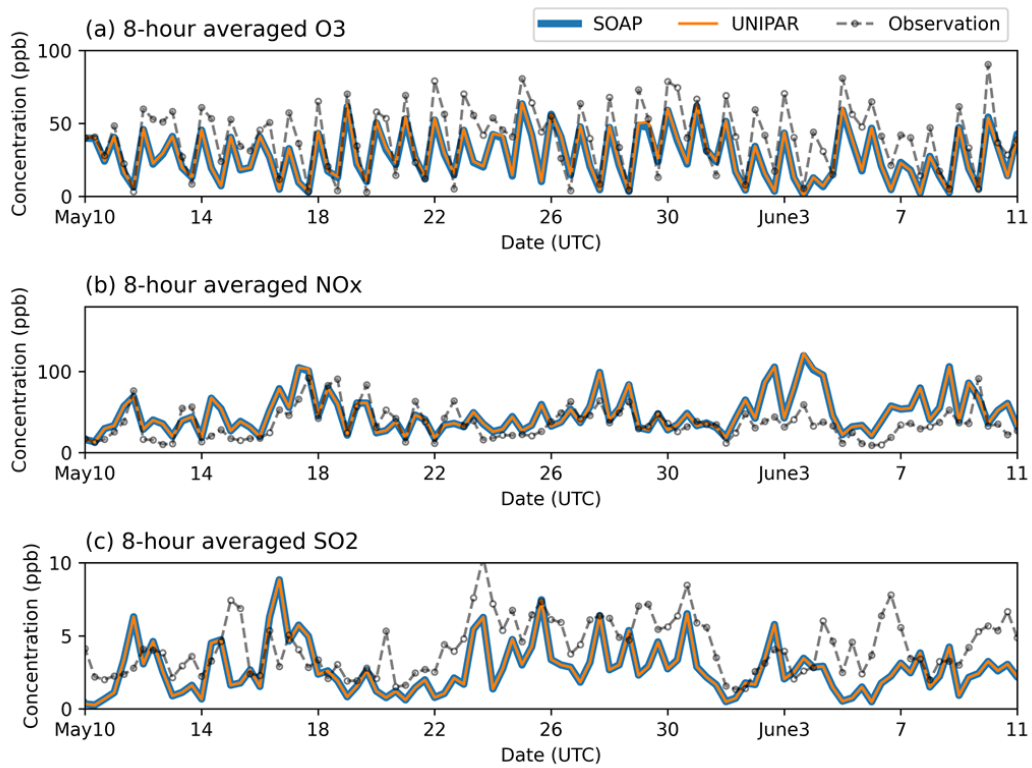


Figure S4. Time profiles of observed and predicted concentrations of (a) 8-hour averaged O₃, (b) 8-hour averaged NO_x, and (c) 8-hour averaged SO₂ at the Olympic Park supersite.

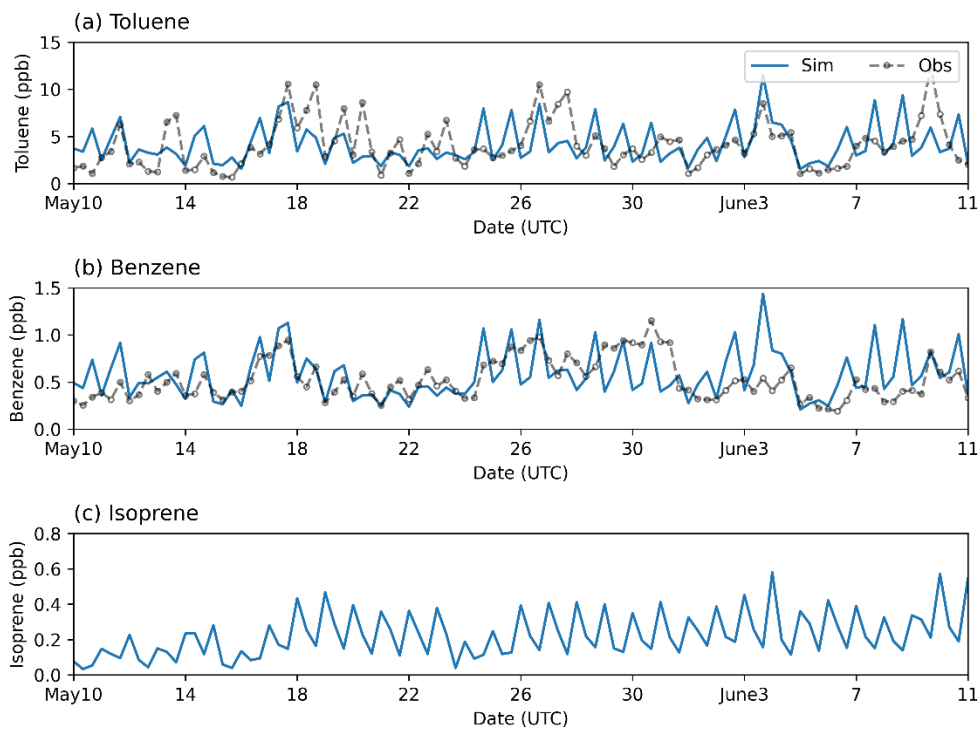


Figure S5. Time profiles of observed and predicted concentrations of (a) 8-hour averaged toluene, (b) 8-hour averaged benzene, and (c) 8-hour averaged isoprene at the Olympic Park supersite. The concentration of toluene and benzene are predicted by using CAMx-UNIPAR.

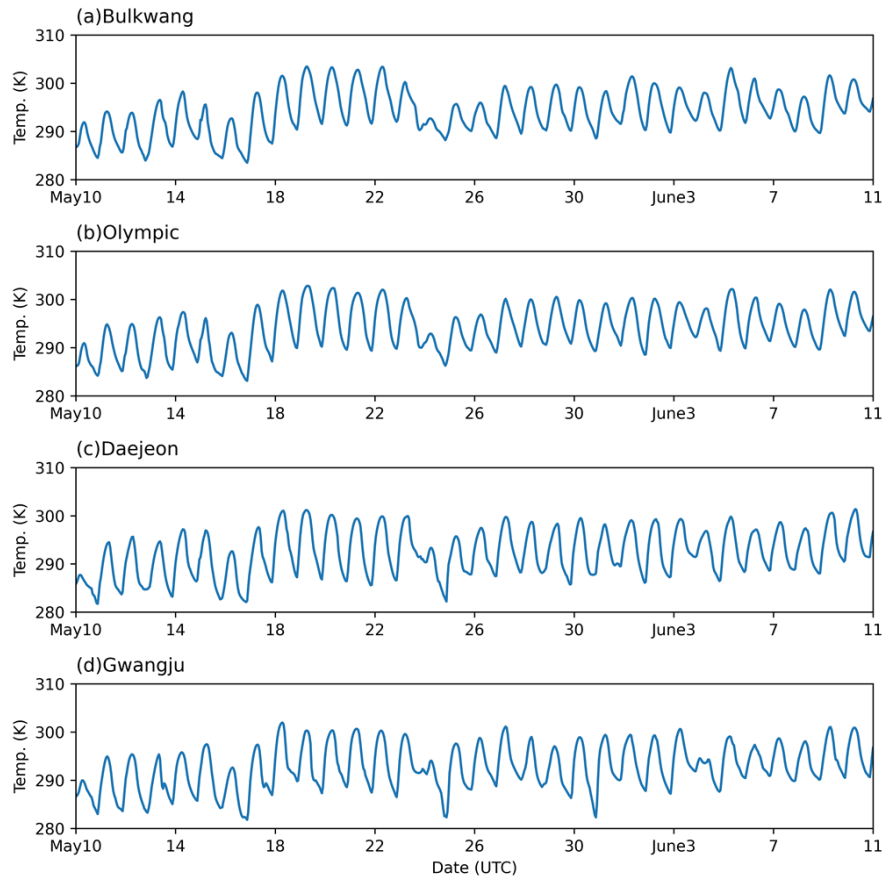


Figure S6. Time profiles of temperature at (a) Bulkwang, (b) Olympic Park, (c) Daejeon, and (d) Gwangju supersites.

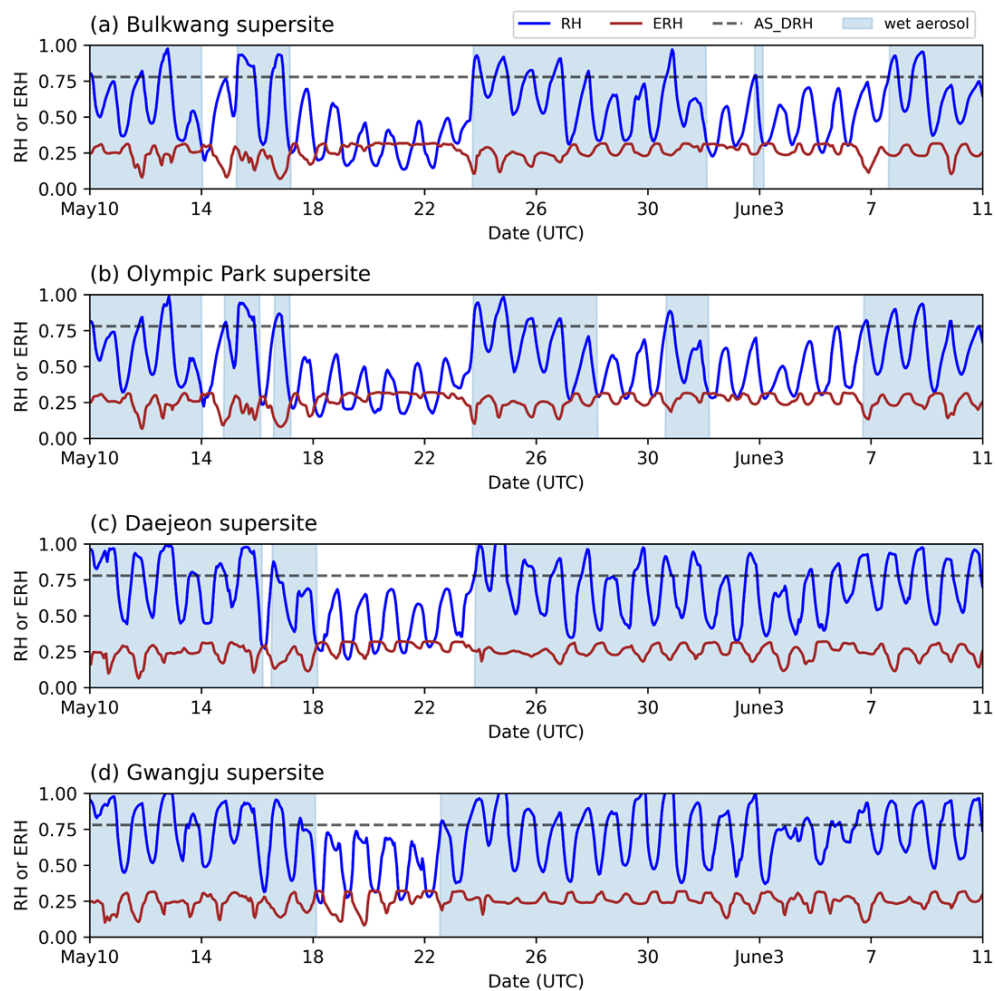


Figure S7. Time profiles of relative humidity (RH), the predicted efflorescence relative humidity (ERH), and aerosol phase state (wet and dry) at (a) Bulkwang, (b) Olympic Park, (c) Daejeon, and (d) Gwangju supersites.

Section S4: Statistic analysis for predictions vs. observations

The statistic parameters analyzed for the relation between predictions and observations include Mean bias error (MBE), the Pearson correlation coefficient (PCC), the mean fractional bias (MFB), mean fractional error (MFE), and the normalized mean bias (NMB). The detailed calculation of each parameter is listed in Table S2.

Table S2. Description of statistic parameters used in this study.

Name	Definition ^a
Observation mean (M_{obs})	$M_{obs} = \frac{1}{N} \sum_{i=1}^N O_i$
Prediction mean (M_{pre})	$M_{pre} = \frac{1}{N} \sum_{i=1}^N Pre_i$
Mean bias error (MBE)	$MBE = \frac{1}{N} \sum_{i=1}^N (Pre_i - O_i)$
Pearson correlation coefficient (PCC)	$PCC = \frac{\sum_{i=1}^N (Pre_i - M_{pre}) \cdot (O_i - M_{obs})}{\sqrt{\sum_{i=1}^N (Pre_i - M_{pre})^2} \cdot \sqrt{\sum_{i=1}^N (O_i - M_{obs})^2}}$
Mean fractional bias (MFB)	$MFB = \frac{1}{N} \sum_{i=1}^N \frac{2 \cdot (Pre_i - O_i)}{Pre_i + O_i}$
Mean fractional error (MFE)	$MFE = \frac{1}{N} \sum_{i=1}^N \frac{2 \cdot Pre_i - O_i }{Pre_i + O_i}$
Normalized mean bias (NMB)	$NMB = \frac{\sum_{i=1}^N (Pre_i - O_i)}{\sum_{i=1}^N O_i}$

^a O_i and Pre_i represent the observation and prediction, respectively.

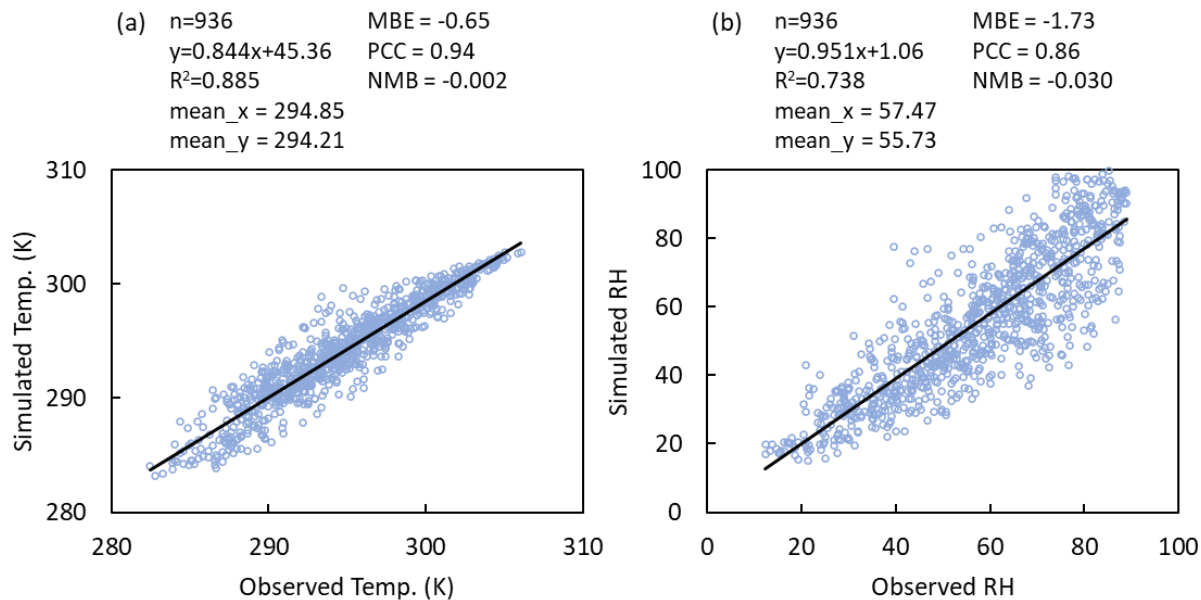


Figure S8. The observed (a) temperature (K) and (b) relative humidity (RH) versus the temperature and RH value from the WRF simulations at the Olympic Park supersite. “MBE”, “PCC”, and “NMB” represent mean bias error, Pearson correlation coefficient, and normalized mean bias, respectively. The detailed equations for the statistic calculation are listed in Table S2.

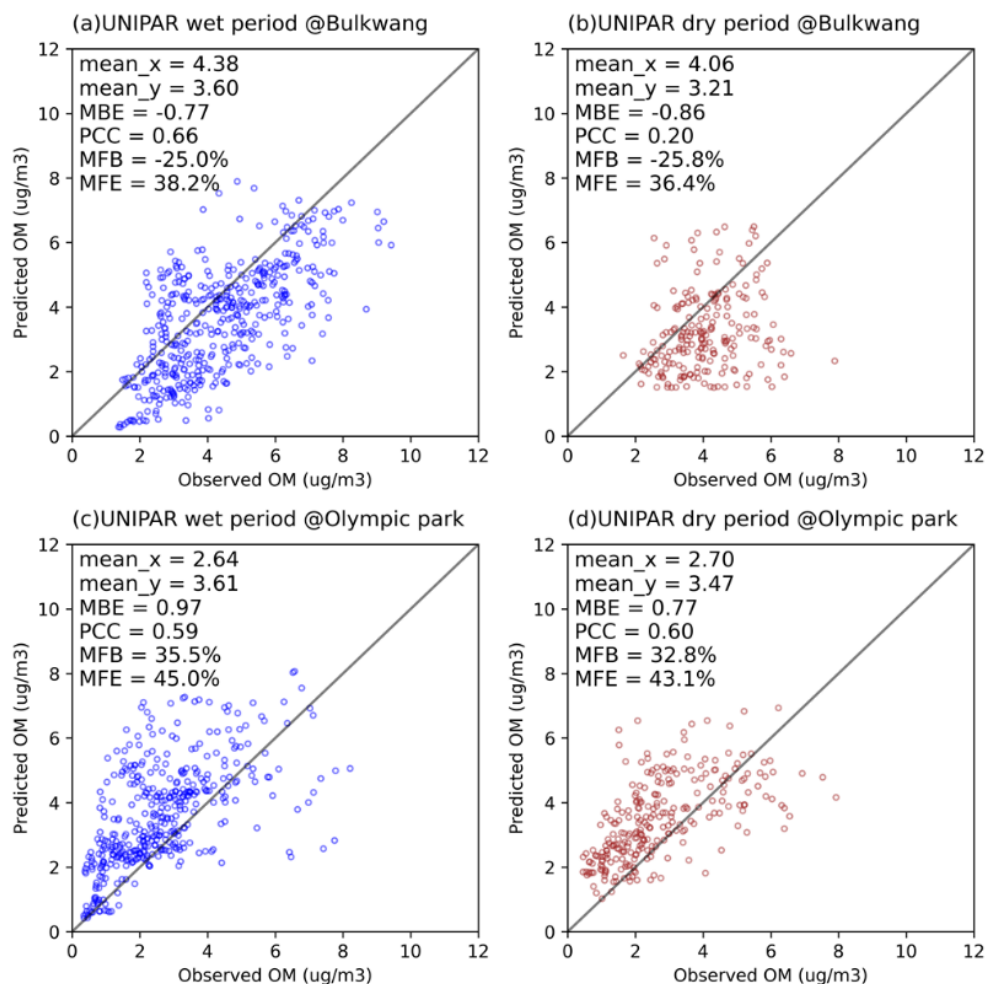


Figure S9. The observation of hourly averaged OM concentrations vs. CAMx-UNIPAR simulation results at the Bulkwang supersite for wet periods (a) and dry periods (b); and the results at the Olympic Park supersite for wet periods (c), and dry periods (d). Terms mean_x and mean_y are the averaged OM concentration of observations and predictions, respectively. MBE is the estimated mean bias error. PCC is the Pearson correlation coefficient. MFB and MFE are the mean fractional bias and mean fractional error, respectively.

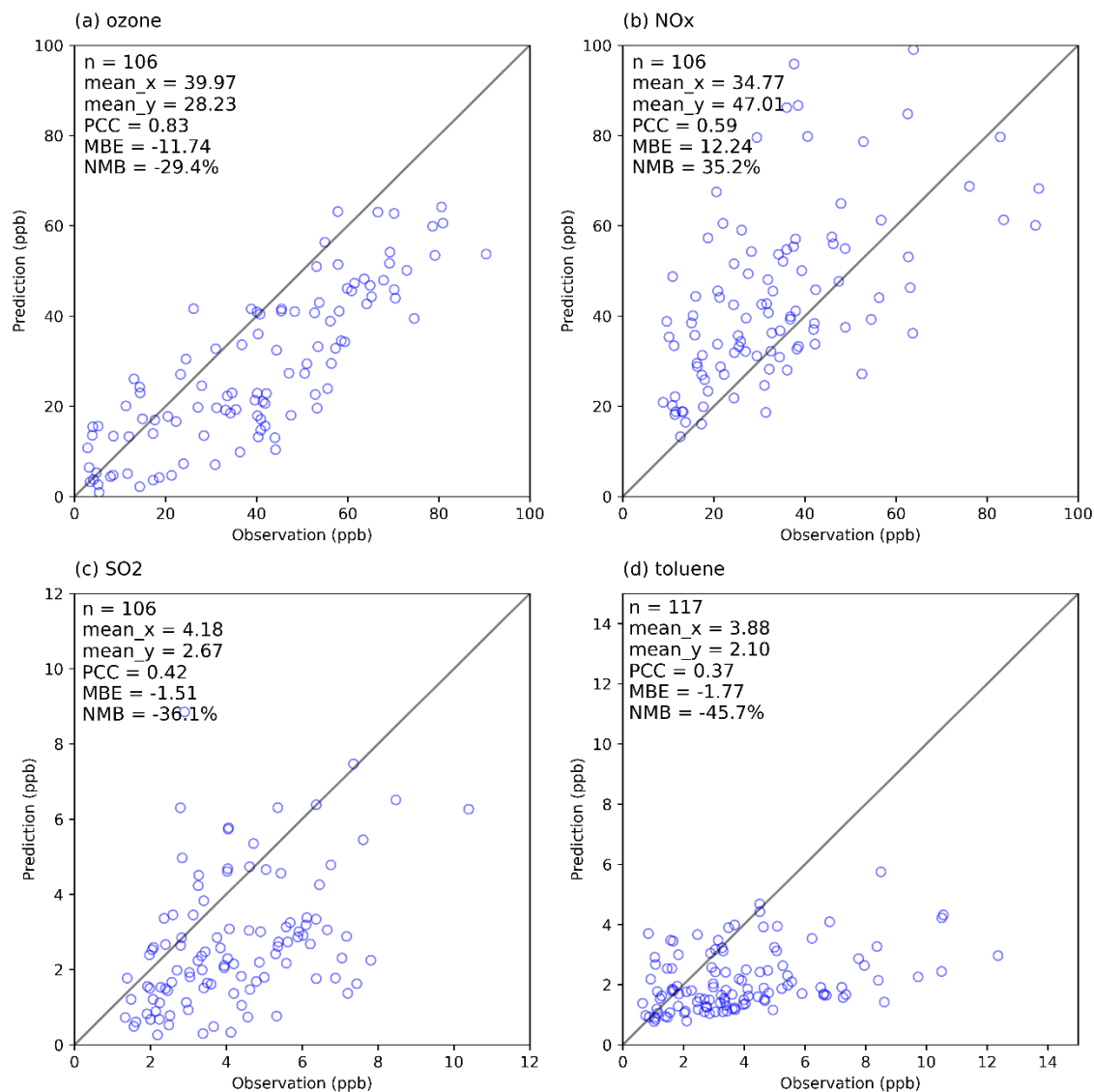


Figure S10. The 8-hour averaged observations vs. simulated concentration (ppb) of (a) ozone, (b) NO_x, (c) SO₂, and (d) toluene at the Olympic Park supersite. The CAMx-UNIPAR was used for the simulation output. Terms “MBE”, “PCC”, and “NMB” represent mean bias error, Pearson correlation coefficient, and normalized mean bias, respectively.

Section S5: Airborne measurements vs. predictions

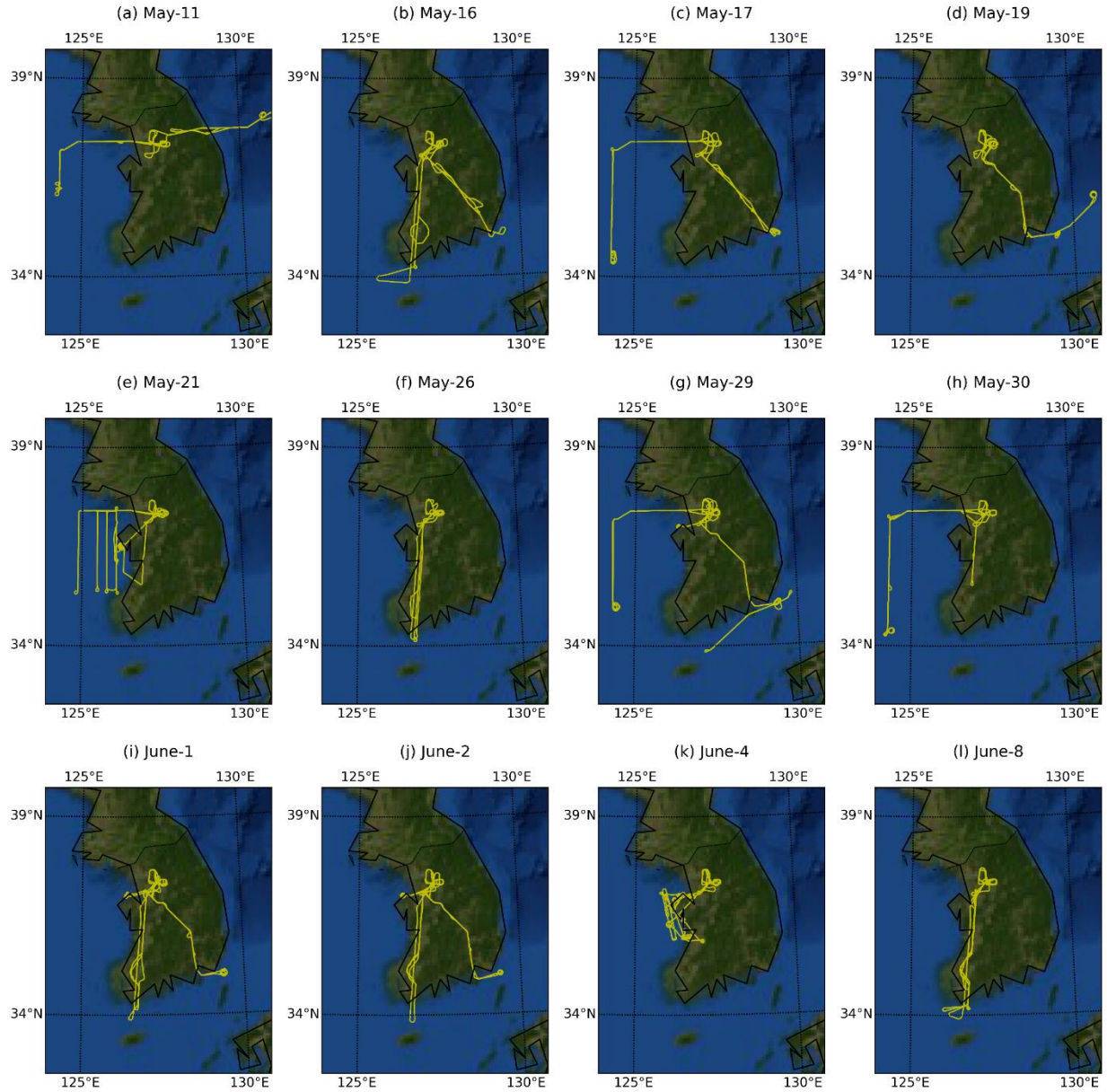


Figure S11. Flight tracks of the NASA DC-8 aircraft missions during the simulated period and regions of this study.

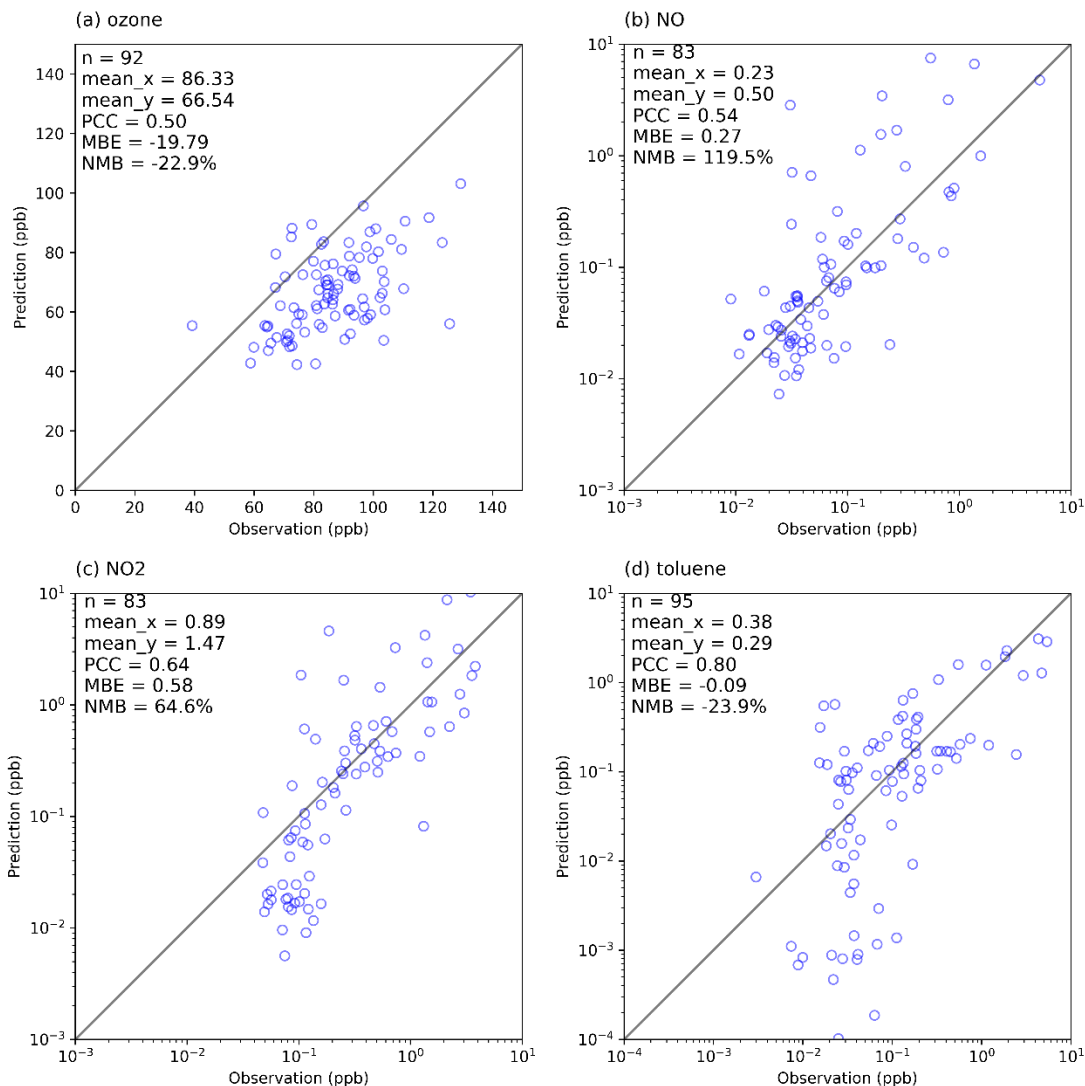


Figure S12. The observations vs. CAMx-UNIPAR simulation results for the concentration (ppb) of (a) ozone, (b) NO, (c) NO₂, and (d) toluene at the whole point during the NASA DC-8 aircraft missions of KORUS-AQ campaign. “PCC”, “MBE”, and “NMB” represent mean bias error, Pearson correlation coefficient, and normalized mean bias, respectively. The detailed equations for the statistic calculation are listed in Table S2.

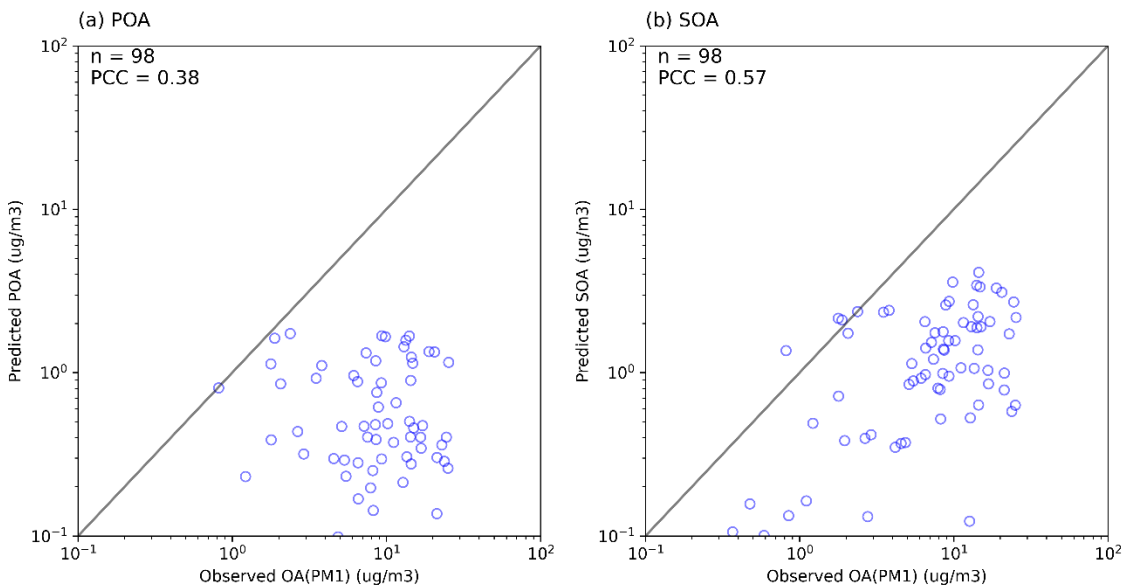


Figure S13. The correlation between the observed organic aerosol (OA) concentration ($\mu\text{g}/\text{m}^3$) and the predicted primary organic aerosol (POA) (a) or the predicted of SOA concentration ($\mu\text{g}/\text{m}^3$) (b). The observed OA data in PM1 were measured by using Aerosol Mass Spectrometer (AMS). Term “PCC” is the Pearson correlation coefficient. The simulated SOA mass is the sum of the OM produced via gas-particle partitioning and heterogeneous reactions of organics by using the UNIPAR module.

Section S6: Spatial distribution of OM concentrations

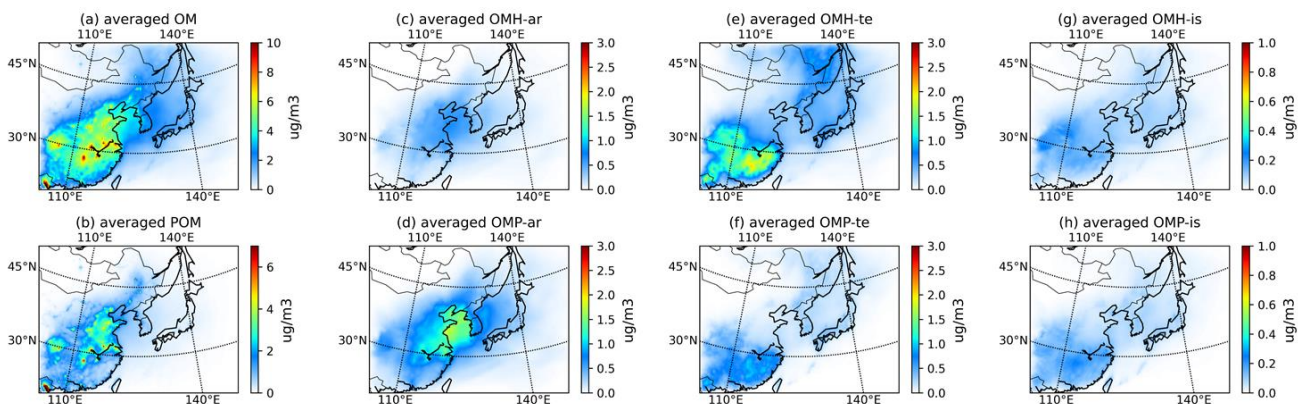


Figure S14. Spatial distribution of episode-averaged concentrations over the East Asian (EA) domain for (a) total OM; (b) primary organic matter (POM); (c) heterogeneously formed aromatic SOA (OMH-ar); (d) partitioned aromatic SOA (OMP-ar); (e) heterogeneously formed terpene SOA (OMH-te); (f) partitioned terpene SOA (OMP-te); (g) heterogeneously formed isoprene SOA (OMH-is); and (h) partitioned isoprene SOA (OMP-is).

Section S7: Model parameters used in CAMx-UNIPAR

Table S3. Stoichiometric coefficient array of oxygenated products for UNIPAR module

Precursor ^a : Benzene	NO _x level: Low	NO _x level: High	Aging stats: Fresh	Aging stats: Old
Lumped Species	A ^b	B ^b	C ^b	D ^b
1VF	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
3VF	-1.62E-05	1.43E-03	-3.75E-02	3.52E-01
4VF	5.07E-06	-4.24E-04	1.09E-02	-4.13E-02
5VF	-9.21E-08	4.36E-06	3.09E-05	1.58E-04
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	1.85E-05	-1.51E-03	3.93E-02	-2.12E-01
8VF	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
2F	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
4F	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
6F	-3.90E-08	3.67E-06	-8.34E-05	8.08E-04
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	1.45E-05	-1.20E-03	3.17E-02	-1.02E-01
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	4.84E-07	-4.49E-05	1.29E-03	-6.91E-03
5M	-1.73E-08	2.10E-06	-3.34E-05	4.11E-04
6M	-1.58E-06	1.33E-04	-3.06E-03	3.74E-02
7M	-1.59E-07	1.31E-05	-3.32E-04	2.89E-03
8M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-4.02E-07	3.29E-05	-8.32E-04	7.11E-03

Lumped Species	A	B	C	D
5S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6S	-9.50E-07	7.74E-05	-1.94E-03	2.80E-02
7S	-8.99E-07	7.35E-05	-1.84E-03	1.96E-02
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6P	-7.34E-06	5.97E-04	-1.48E-02	1.96E-01
7P	-1.32E-05	1.08E-03	-2.82E-02	2.81E-01
8P	2.30E-05	-1.87E-03	4.67E-02	3.24E-01
1MA	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
3MA	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
5MA	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
7MA	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
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	6.25E-06	-5.14E-04	1.37E-02	1.46E-01

^a The high NO_x level and the low NO_x level are the VOC to NO_x ratio lower than 5 ppbC/ppb and higher than 5 ppbC/ppb, respectively. The fresh and aging status are the moment when 20% of precursor was consumed and when 100% of precursor was consumed.

^b The stoichiometric coefficient is calculated by $\alpha = A \times (VOC:NO_x)^3 + B \times (VOC:NO_x)^2 + C \times (VOC:NO_x) + D$, where VOC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S3. (Continued)

Precursor: Toluene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	6.87E-08	-7.11E-06	2.15E-04	-5.89E-04
3VF	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
5VF	-1.54E-07	1.57E-05	-3.67E-04	3.05E-03
6VF	-3.91E-08	6.62E-06	-1.72E-04	1.49E-03
7VF	2.65E-07	-2.81E-05	8.03E-04	7.40E-03
8VF	-1.33E-08	2.28E-06	-1.71E-04	1.97E-02
1F	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
3F	-5.37E-07	5.15E-05	-1.10E-03	1.34E-02
4F	-2.35E-07	2.93E-05	-6.95E-04	6.13E-03
5F	-7.60E-08	6.65E-06	-1.43E-04	9.38E-04
6F	1.44E-07	-1.89E-05	7.96E-04	2.69E-03
7F	1.21E-06	-1.25E-04	3.14E-03	6.33E-02
8F	2.47E-06	-2.44E-04	6.15E-03	3.42E-02
1M	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
3M	4.84E-07	-5.25E-05	1.67E-03	-7.22E-03
4M	-1.81E-07	-3.78E-07	6.41E-04	1.38E-02
5M	2.78E-07	-3.36E-05	1.31E-03	3.16E-03
6M	5.05E-07	-9.49E-05	4.18E-03	2.68E-02
7M	9.01E-07	-9.08E-05	1.76E-03	5.30E-02
8M	1.27E-06	-1.26E-04	2.91E-03	8.34E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-2.84E-08	2.56E-06	-5.57E-05	3.59E-04
3S	-1.34E-08	1.44E-06	-3.45E-05	2.39E-04
4S	1.22E-07	-1.68E-05	7.28E-04	-1.62E-03
5S	-1.76E-06	2.24E-04	-5.74E-03	7.71E-02
6S	1.55E-06	-1.15E-04	3.94E-03	4.27E-02
7S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-2.35E-07	1.92E-05	-4.05E-04	2.56E-03
2P	-5.77E-07	5.43E-05	-1.20E-03	7.79E-03
3P	-4.69E-07	4.06E-05	-9.53E-05	7.87E-02
4P	-6.81E-06	6.54E-04	-1.55E-02	1.74E-01
5P	9.30E-07	-1.39E-04	5.98E-03	3.19E-02
6P	-8.50E-07	1.05E-04	-4.45E-03	1.09E-01
7P	-1.90E-06	2.09E-04	-7.09E-03	1.92E-01
8P	2.43E-07	-2.30E-05	-1.24E-03	1.47E-01
1MA	-1.47E-07	1.66E-05	-3.95E-04	2.70E-03
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	4.01E-06	-4.13E-04	1.20E-02	4.90E-02
GLY	3.41E-06	-3.44E-04	9.28E-03	1.78E-01

Table S3. (Continued)

Precursor: o-Xylene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	1.11E-07	-1.46E-05	5.82E-04	-2.22E-03
3VF	-1.60E-07	1.37E-05	-2.97E-04	1.12E-02
4VF	-1.51E-07	1.38E-05	-3.31E-04	3.55E-03
5VF	-1.12E-07	1.07E-05	-3.19E-04	5.34E-03
6VF	-4.17E-08	3.86E-06	-1.18E-04	2.07E-03
7VF	4.48E-06	-3.98E-04	1.04E-02	1.02E-01
8VF	-3.60E-07	3.31E-05	-8.26E-04	2.94E-02
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	3.59E-07	-7.74E-05	4.42E-03	-1.08E-02
5F	-3.38E-07	2.31E-05	-2.50E-04	5.21E-03
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	2.40E-07	-2.55E-05	6.93E-04	1.39E-02
8F	1.10E-06	-1.01E-04	2.63E-03	9.03E-03
1M	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
3M	-1.87E-07	1.30E-05	-2.11E-04	3.41E-03
4M	-1.53E-07	1.46E-05	-3.61E-04	2.66E-03
5M	4.45E-08	-8.88E-06	4.47E-04	-8.34E-04
6M	-3.32E-07	4.92E-06	1.37E-03	3.66E-03
7M	5.14E-07	-5.42E-05	1.53E-03	7.76E-02
8M	2.18E-06	-1.93E-04	4.61E-03	4.05E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-4.23E-08	4.01E-06	-9.94E-05	7.34E-04
3S	-2.20E-08	2.08E-06	-5.20E-05	3.87E-04
4S	-6.37E-09	6.26E-07	-1.56E-05	1.15E-04
5S	1.14E-07	-1.31E-05	4.22E-04	2.60E-02
6S	-7.94E-08	-3.26E-05	3.19E-03	5.73E-03
7S	-1.67E-07	1.00E-05	-1.35E-04	1.31E-02
8S	1.03E-06	-1.04E-04	2.91E-03	1.22E-01
1P	-5.51E-08	4.93E-06	-1.22E-04	9.07E-04
2P	-2.73E-07	2.60E-05	-6.51E-04	4.84E-03
3P	-6.35E-07	3.60E-05	-1.34E-04	5.80E-02
4P	-7.97E-07	1.06E-04	-2.62E-03	1.03E-01
5P	-1.18E-06	7.95E-05	-9.47E-04	5.77E-02
6P	-3.70E-07	3.64E-05	-1.02E-03	2.16E-02
7P	1.88E-06	-1.19E-04	5.96E-04	1.74E-01
8P	1.70E-06	-1.48E-04	3.74E-03	9.30E-02
1MA	-5.74E-08	5.30E-06	-1.31E-04	9.74E-04
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	3.18E-06	-3.01E-04	8.00E-03	6.15E-02
GLY	3.57E-07	-4.46E-05	1.40E-03	6.18E-02

Table S3. (Continued)

Precursor: m-Xylene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	-1.11E-08	1.54E-06	-5.43E-05	7.70E-04
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	-1.99E-07	1.62E-05	-5.27E-04	3.16E-02
8VF	-2.52E-07	2.42E-05	-7.40E-04	3.95E-02
1F	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
3F	-2.77E-07	3.24E-05	-9.01E-04	3.19E-02
4F	-5.67E-08	7.99E-06	-2.45E-04	4.64E-03
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	-7.13E-08	3.53E-06	7.00E-05	4.08E-03
7F	1.14E-06	-1.53E-04	5.89E-03	1.93E-01
8F	5.72E-07	-7.52E-05	2.38E-03	3.40E-02
1M	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
3M	-3.16E-08	2.41E-06	-4.81E-05	1.03E-03
4M	-2.31E-07	-1.33E-06	1.51E-03	9.83E-03
5M	4.02E-10	7.36E-08	-2.63E-06	1.43E-04
6M	-1.36E-07	5.29E-06	4.69E-04	5.32E-03
7M	-4.84E-07	3.90E-05	-1.14E-03	7.82E-02
8M	7.15E-07	-9.35E-05	2.80E-03	6.24E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-7.29E-09	2.89E-07	9.37E-06	4.19E-04
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5S	-1.69E-07	2.58E-05	-6.41E-04	3.62E-02
6S	-6.21E-07	3.15E-05	1.06E-03	3.94E-02
7S	-6.06E-08	5.01E-06	-1.41E-04	7.59E-03
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-3.33E-09	3.66E-07	-8.46E-06	5.55E-05
2P	-7.44E-08	1.38E-05	-3.46E-04	2.37E-03
3P	-4.89E-07	4.15E-05	-1.01E-03	3.57E-02
4P	2.42E-08	1.58E-05	2.41E-04	8.51E-02
5P	-3.89E-07	3.12E-05	-6.29E-04	3.41E-02
6P	-2.93E-07	4.37E-05	-2.01E-03	4.72E-02
7P	3.19E-07	-3.66E-05	5.40E-04	2.77E-01
8P	-1.52E-07	1.75E-05	-4.92E-04	1.35E-02
1MA	-1.74E-09	2.63E-07	-5.99E-06	3.73E-05
2MA	-2.06E-10	2.66E-07	-7.35E-06	5.29E-05
3MA	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
5MA	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
7MA	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
MGLY	2.33E-07	-8.70E-05	2.92E-03	2.22E-01
GLY	-8.13E-08	-1.79E-06	1.07E-04	5.80E-02

Table S3. (Continued)

Precursor: p-Xylene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	-3.70E-06	3.32E-04	-9.14E-03	1.53E-01
8VF	-1.31E-06	1.14E-04	-2.47E-03	3.58E-02
1F	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
3F	-8.40E-07	7.52E-05	-1.92E-03	2.23E-02
4F	-1.43E-07	1.14E-05	-2.98E-04	1.09E-02
5F	5.00E-08	-4.69E-06	1.37E-04	-5.67E-04
6F	-6.20E-07	6.27E-05	-2.14E-03	3.61E-02
7F	-3.02E-06	2.67E-04	-6.54E-03	6.36E-02
8F	-8.18E-07	7.27E-05	-1.86E-03	1.79E-02
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-7.03E-07	6.93E-05	-2.64E-03	6.26E-02
5M	-1.07E-08	1.22E-06	-4.38E-05	9.25E-04
6M	-1.61E-06	1.34E-04	-2.81E-03	4.29E-02
7M	-3.02E-06	2.76E-04	-7.75E-03	1.68E-01
8M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	4.58E-09	-2.91E-07	-1.46E-05	1.63E-03
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	7.06E-07	-7.08E-05	2.38E-03	-3.64E-03
5S	-1.57E-06	1.90E-04	-8.23E-03	1.95E-01
6S	-1.08E-06	9.91E-05	-2.82E-03	3.96E-02
7S	-1.22E-07	9.34E-06	-2.53E-04	7.17E-03
8S	-1.11E-05	9.78E-04	-2.29E-02	2.45E-01
1P	1.76E-06	-1.67E-04	4.66E-03	-2.85E-02
2P	-1.25E-07	7.62E-06	1.23E-04	1.72E-03
3P	-2.64E-06	2.37E-04	-5.66E-03	6.66E-02
4P	-2.86E-07	-2.42E-06	3.97E-03	2.26E-02
5P	-8.95E-07	9.68E-05	-3.95E-03	1.22E-01
6P	2.44E-06	-2.31E-04	6.75E-03	3.84E-03
7P	-4.23E-06	3.75E-04	-8.17E-03	9.04E-02
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	4.43E-08	-5.49E-06	2.24E-04	-1.39E-03
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-7.96E-06	7.20E-04	-1.96E-02	2.15E-01
GLY	-8.91E-06	8.03E-04	-2.12E-02	2.63E-01

Table S3. (Continued)

Precursor: 123-TMB^a NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	8.59E-08	-9.74E-06	3.35E-04	-3.01E-03
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	1.30E-06	-1.39E-04	4.19E-03	-1.41E-02
8VF	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
2F	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
4F	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
6F	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
8F	1.98E-06	-2.13E-04	6.48E-03	-2.72E-02
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	1.24E-06	-1.41E-04	4.90E-03	-4.41E-02
3M	5.30E-07	-5.63E-05	1.69E-03	-7.12E-03
4M	1.01E-06	-1.13E-04	3.84E-03	-3.43E-02
5M	1.06E-06	-1.12E-04	3.45E-03	-2.57E-02
6M	-9.24E-06	9.87E-04	-3.04E-02	4.66E-01
7M	2.90E-06	-3.16E-04	9.48E-03	6.11E-02
8M	-9.68E-06	1.06E-03	-3.42E-02	4.02E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	3.42E-07	-3.63E-05	1.13E-03	-8.67E-03
4S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5S	6.30E-06	-7.05E-04	2.33E-02	-1.46E-01
6S	5.10E-06	-5.74E-04	1.89E-02	-9.50E-02
7S	1.14E-06	-1.22E-04	3.74E-03	-2.35E-02
8S	1.12E-06	-1.11E-04	2.37E-03	2.80E-01
1P	1.98E-07	-2.31E-05	8.34E-04	-7.62E-03
2P	-4.37E-07	4.60E-05	-1.54E-03	2.21E-02
3P	1.78E-06	-2.00E-04	6.77E-03	-6.05E-02
4P	-2.99E-06	2.84E-04	-5.81E-03	1.90E-01
5P	7.03E-06	-7.44E-04	2.29E-02	-1.65E-01
6P	-1.15E-06	1.28E-04	-4.10E-03	6.67E-02
7P	-4.33E-06	4.69E-04	-1.53E-02	2.32E-01
8P	-5.99E-06	6.43E-04	-2.03E-02	2.90E-01
1MA	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
3MA	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
5MA	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
7MA	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
MGLY	-2.72E-06	2.99E-04	-1.01E-02	1.91E-01
GLY	2.41E-08	-3.72E-06	-6.28E-05	4.59E-02

^a “123-TMB” represents 1,2,3-trimethylbenzene.

Table S3. (Continued)

Precursor: 124-TMB^a NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	-1.62E-07	2.84E-05	-1.32E-03	5.05E-02
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	4.75E-08	-3.17E-07	-1.11E-05	2.67E-04
3F	-4.18E-08	5.35E-06	-2.37E-04	8.75E-03
4F	7.85E-09	4.83E-07	-3.22E-05	7.78E-04
5F	-7.98E-08	1.16E-05	-4.88E-04	1.10E-02
6F	1.07E-06	-1.72E-04	7.40E-03	1.99E-01
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	9.43E-08	-1.85E-05	7.90E-04	7.87E-03
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-9.05E-08	1.26E-05	-4.10E-04	3.05E-02
5M	-5.77E-08	7.54E-06	-2.51E-04	8.62E-03
6M	-4.16E-08	6.38E-06	-2.30E-04	9.87E-03
7M	-4.49E-07	5.94E-05	-2.55E-03	1.42E-01
8M	2.68E-07	-5.18E-05	2.22E-03	1.98E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	-2.97E-09	4.10E-07	-1.52E-05	2.60E-04
4S	3.31E-08	-5.89E-07	2.28E-06	1.03E-04
5S	-1.64E-07	2.75E-05	-1.28E-03	4.49E-02
6S	-7.04E-08	1.36E-05	-4.05E-04	3.10E-02
7S	-8.25E-08	1.10E-05	-4.78E-04	1.50E-02
8S	9.98E-08	-2.61E-05	8.46E-04	2.56E-01
1P	2.02E-08	-6.51E-07	7.93E-06	-6.17E-06
2P	-2.98E-08	3.68E-06	-1.46E-04	3.83E-03
3P	1.50E-08	-4.47E-07	5.62E-06	4.52E-06
4P	7.64E-07	-6.40E-05	2.51E-03	1.17E-01
5P	-4.89E-08	6.94E-06	-2.99E-04	8.33E-03
6P	7.34E-08	-5.10E-06	-1.04E-04	4.95E-02
7P	8.78E-08	-2.16E-05	8.20E-04	1.27E-01
8P	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
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	1.94E-07	-6.93E-05	3.02E-03	1.45E-01
GLY	-4.54E-10	-3.27E-06	1.21E-04	3.14E-02

^a “124-TMB” represents 1,2,4-trimethylbenzene.

Table S3. (Continued)

Precursor: 135-TMB NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	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
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-2.47E-07	2.56E-05	-6.57E-04	5.06E-03
3F	-4.30E-08	5.17E-06	-2.15E-04	5.05E-03
4F	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
6F	2.11E-06	-2.36E-04	7.67E-03	6.51E-02
7F	-3.51E-08	3.57E-06	-8.98E-05	6.85E-04
8F	-5.55E-07	6.46E-05	-2.14E-03	3.78E-02
1M	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
3M	-8.02E-09	8.36E-07	-2.17E-05	1.67E-04
4M	-1.54E-07	1.56E-05	-3.89E-04	3.12E-03
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7M	-9.59E-07	1.08E-04	-3.80E-03	9.51E-02
8M	4.82E-06	-5.28E-04	1.57E-02	8.49E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-1.27E-06	1.47E-04	-4.89E-03	8.07E-02
5S	-1.94E-07	2.13E-05	-5.68E-04	4.51E-03
6S	-5.28E-07	5.59E-05	-1.61E-03	2.27E-02
7S	-2.06E-07	2.44E-05	-9.67E-04	2.09E-02
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-2.10E-07	2.26E-05	-6.09E-04	4.77E-03
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	-3.34E-07	3.60E-05	-9.63E-04	7.55E-03
4P	-2.06E-06	2.22E-04	-4.27E-03	2.08E-01
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6P	-7.78E-07	9.57E-05	-3.32E-03	1.12E-01
7P	1.55E-06	-1.58E-04	4.34E-03	2.73E-01
8P	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
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	3.57E-06	-3.81E-04	9.37E-03	3.30E-01
GLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00

^a “135-TMB” represents 1,3,5-trimethylbenzene.

Table S3. (Continued)

Precursor: Ethylbenzene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	8.09E-08	-5.16E-06	1.07E-04	-6.63E-04
2VF	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
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	-5.31E-08	3.69E-06	-8.82E-05	1.75E-03
6VF	9.83E-08	-7.49E-06	8.84E-05	9.87E-03
7VF	-3.36E-09	2.89E-07	-2.41E-06	-5.33E-06
8VF	-2.12E-07	1.61E-05	-3.64E-04	1.49E-02
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	1.05E-07	-8.05E-06	8.05E-05	1.17E-02
3F	-8.36E-09	3.47E-06	2.62E-04	-3.32E-03
4F	-2.84E-07	2.36E-05	-3.71E-04	4.90E-03
5F	-3.44E-08	2.09E-06	-3.29E-06	-1.07E-04
6F	2.24E-06	-1.56E-04	3.28E-03	2.24E-02
7F	9.69E-07	-7.35E-05	7.39E-04	7.80E-02
8F	1.63E-06	-1.23E-04	2.43E-03	1.61E-02
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-4.19E-08	3.10E-06	-5.32E-05	2.89E-04
3M	-6.51E-07	2.98E-05	-2.52E-04	1.40E-02
4M	1.58E-06	-1.00E-04	2.23E-03	-1.51E-02
5M	-2.66E-07	1.79E-05	-2.84E-04	1.72E-03
6M	3.58E-06	-2.26E-04	4.67E-03	-3.00E-02
7M	4.52E-07	-3.93E-05	7.03E-04	5.06E-02
8M	8.10E-06	-6.35E-04	1.30E-02	1.55E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	2.74E-07	1.45E-05	8.48E-04	1.68E-02
5S	1.03E-05	-6.71E-04	1.43E-02	-7.64E-02
6S	-4.06E-08	2.91E-06	-9.05E-05	6.66E-03
7S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-5.81E-07	3.87E-05	-4.36E-04	9.84E-04
2P	-5.72E-07	3.60E-05	-4.79E-04	2.35E-03
3P	-1.09E-06	1.10E-04	-3.08E-03	1.13E-01
4P	9.96E-07	-5.14E-05	3.66E-03	1.05E-02
5P	1.62E-06	-1.09E-04	2.81E-03	6.20E-03
6P	-4.10E-07	3.45E-05	-4.21E-04	1.11E-02
7P	-9.34E-06	6.63E-04	-1.60E-02	4.28E-01
8P	-1.19E-05	8.09E-04	-1.55E-02	2.89E-01
1MA	-1.80E-07	1.31E-05	-1.67E-04	5.84E-04
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	5.32E-07	-6.40E-05	1.08E-03	2.17E-01

Table S3. (Continued)

Precursor: Propylbenzene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	2.41E-08	-1.66E-06	4.72E-05	-4.07E-04
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	1.97E-07	-1.80E-05	5.67E-04	-3.76E-03
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	-1.19E-07	1.02E-05	-2.72E-04	5.09E-03
7VF	1.84E-07	-1.64E-05	4.74E-04	-3.33E-03
8VF	-5.09E-09	8.23E-07	-2.89E-06	4.39E-03
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	9.34E-09	-1.80E-06	1.42E-04	2.61E-03
3F	2.19E-07	-1.95E-05	6.24E-04	-4.16E-03
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	2.30E-08	-2.30E-06	8.66E-05	-7.96E-04
6F	-2.79E-06	2.36E-04	-6.39E-03	1.33E-01
7F	-2.88E-07	2.31E-05	-8.28E-04	3.90E-02
8F	-1.61E-06	1.34E-04	-3.53E-03	5.33E-02
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	2.01E-08	-1.89E-06	6.14E-05	-5.31E-04
3M	3.49E-06	-3.21E-04	9.13E-03	-6.19E-02
4M	1.07E-07	-1.02E-05	3.31E-04	-2.41E-03
5M	1.84E-07	-1.77E-05	6.92E-04	-6.20E-03
6M	2.64E-07	-2.45E-05	8.43E-04	-7.19E-03
7M	-3.05E-06	2.45E-04	-6.38E-03	1.21E-01
8M	-1.66E-06	1.00E-04	-1.75E-03	1.58E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	2.51E-08	-2.21E-06	6.63E-05	-5.45E-04
3S	8.00E-08	-7.29E-06	2.18E-04	-1.77E-03
4S	1.32E-06	-1.19E-04	4.72E-03	-1.90E-02
5S	1.67E-06	-1.62E-04	4.96E-03	-2.47E-02
6S	5.77E-08	-5.25E-06	1.40E-04	4.68E-03
7S	-3.06E-07	2.40E-05	-6.67E-04	4.96E-02
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	8.93E-07	-8.54E-05	2.81E-03	-2.47E-02
2P	7.31E-07	-5.30E-05	1.11E-03	8.07E-02
3P	-1.37E-06	9.88E-05	-7.29E-05	2.99E-02
4P	-4.93E-07	4.97E-05	-1.21E-03	1.58E-02
5P	1.67E-07	-1.52E-05	4.23E-04	-3.11E-03
6P	-7.32E-06	6.53E-04	-1.76E-02	2.53E-01
7P	-1.85E-06	1.69E-04	-5.10E-03	2.67E-01
8P	5.43E-06	-4.83E-04	1.28E-02	-9.61E-03
1MA	2.98E-07	-2.70E-05	8.30E-04	-7.04E-03
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	4.07E-07	-6.35E-05	2.07E-03	1.69E-01

Table S3. (Continued)

Precursor: Terpene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	-1.25E-07	9.33E-06	-6.15E-05	2.75E-05
2VF	-1.63E-10	-1.74E-08	2.01E-06	-1.27E-05
3VF	7.41E-08	-6.44E-06	1.40E-04	-6.48E-05
4VF	-1.77E-09	4.96E-08	4.85E-06	-3.40E-05
5VF	6.08E-08	-7.17E-06	2.45E-04	5.53E-03
6VF	4.10E-09	-3.24E-07	4.87E-06	9.13E-05
7VF	9.10E-08	-7.97E-06	2.02E-04	6.39E-05
8VF	-1.20E-08	7.30E-07	2.30E-06	-2.69E-05
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-9.71E-09	1.04E-06	2.85E-06	8.45E-06
5F	-6.16E-08	4.90E-06	-4.75E-05	6.01E-04
6F	-2.29E-08	1.68E-06	-1.05E-05	4.15E-04
7F	1.86E-07	-1.49E-05	1.53E-04	1.38E-02
8F	1.32E-09	-6.58E-08	3.68E-06	6.51E-05
1M	-7.28E-07	6.14E-05	-7.32E-04	2.44E-03
2M	3.02E-07	-2.90E-05	8.51E-04	-2.53E-03
3M	-8.02E-07	6.28E-05	-4.52E-04	4.82E-04
4M	-1.77E-06	1.34E-04	-5.57E-04	4.20E-02
5M	1.79E-06	-1.83E-04	5.50E-03	3.51E-02
6M	1.37E-06	-8.33E-05	-1.90E-03	4.68E-01
7M	8.67E-07	-6.62E-05	6.31E-04	6.38E-02
8M	-3.68E-08	2.72E-06	-1.12E-05	-2.19E-05
1S	-2.33E-07	8.99E-06	6.79E-04	2.84E-03

Lumped Species	A	B	C	D
2S	2.27E-07	-2.50E-05	1.04E-03	3.71E-03
3S	1.06E-06	-1.08E-04	3.33E-03	6.34E-03
4S	4.62E-06	-4.27E-04	1.11E-02	4.03E-02
5S	2.30E-06	-1.93E-04	3.71E-03	4.09E-02
6S	-1.08E-06	7.90E-05	-4.63E-04	9.47E-03
7S	-9.86E-08	6.17E-06	-8.14E-06	1.55E-03
8S	-1.66E-10	-1.20E-09	1.23E-06	-7.86E-06
1P	-2.22E-07	1.67E-05	-1.15E-04	2.47E-03
2P	6.43E-07	-6.84E-05	2.28E-03	-6.95E-03
3P	-3.70E-08	2.34E-06	2.02E-05	-2.10E-04
4P	-5.36E-07	4.61E-05	-7.33E-04	1.19E-02
5P	-1.48E-06	1.24E-04	-2.36E-03	1.59E-01
6P	2.78E-08	-2.34E-06	4.13E-05	9.63E-04
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8P	1.77E-06	-1.54E-04	3.40E-03	3.69E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	4.84E-09	-1.65E-07	-2.14E-05	1.46E-03
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	-3.10E-09	1.24E-07	8.61E-06	-5.64E-05
5MA	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
7MA	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
MGLY	-2.92E-08	3.52E-06	-1.50E-04	2.57E-03
GLY	3.72E-08	-3.37E-06	8.99E-05	-2.77E-05

Table S3. (Continued)

Precursor: Isoprene NO_x level: Low NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	2.09E-10	-1.91E-08	5.24E-07	-3.41E-06
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	2.25E-13	-2.09E-11	5.96E-10	-4.21E-09
7VF	1.04E-06	-9.24E-05	2.29E-03	-4.93E-03
8VF	2.09E-08	-1.86E-06	4.60E-05	-2.82E-05
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	3.52E-08	-3.41E-06	1.05E-04	-3.05E-04
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	-1.34E-07	1.62E-05	-6.64E-04	9.79E-03
7F	2.74E-07	-2.68E-05	8.42E-04	-2.77E-03
8F	-1.37E-08	1.08E-06	-2.17E-05	2.49E-04
1M	7.04E-09	-6.53E-07	1.90E-05	-1.12E-04
2M	2.25E-08	-2.14E-06	6.03E-05	-1.43E-04
3M	2.95E-07	-2.74E-05	7.58E-04	-3.44E-04
4M	3.76E-10	-1.81E-08	-4.36E-07	3.07E-05
5M	8.14E-08	-7.57E-06	2.23E-04	-1.42E-06
6M	-1.37E-07	4.34E-06	6.14E-04	6.92E-03
7M	-6.86E-07	5.46E-05	-1.07E-03	1.49E-02
8M	2.46E-07	1.37E-05	-2.83E-03	1.43E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-1.06E-13	1.14E-11	-3.93E-10	4.48E-09
3S	-8.40E-11	1.18E-08	-5.54E-07	9.49E-06
4S	5.61E-09	8.12E-08	-3.91E-05	1.14E-03
5S	3.36E-08	-2.88E-06	7.96E-05	1.56E-03
6S	5.06E-07	-4.39E-05	1.17E-03	1.74E-02
7S	2.27E-09	3.09E-06	-2.64E-04	8.49E-03
8S	5.91E-07	-5.41E-05	1.49E-03	1.14E-02
1P	1.89E-07	-1.79E-05	5.09E-04	-1.12E-03
2P	2.67E-07	-2.27E-05	4.74E-04	4.87E-03
3P	3.14E-08	-2.85E-06	7.30E-05	-1.80E-04
4P	-2.55E-08	2.09E-06	-4.22E-05	5.23E-04
5P	-1.21E-08	1.69E-06	-8.72E-05	1.90E-03
6P	-4.49E-07	4.52E-05	-1.45E-03	2.07E-02
7P	-2.08E-06	1.66E-04	-2.65E-03	3.47E-02
8P	-7.89E-07	1.06E-04	-4.70E-03	9.99E-02
1MA	6.47E-09	-6.00E-07	1.61E-05	-2.39E-05
2MA	1.03E-08	-9.70E-07	2.77E-05	-1.08E-04
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	-4.67E-10	3.86E-08	-6.91E-07	4.62E-06
5MA	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
7MA	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
MGLY	-1.35E-07	1.74E-05	-8.43E-04	2.14E-02
GLY	-4.19E-08	6.53E-06	-3.99E-04	1.23E-02
IEPOX	1.59E-06	-1.60E-04	5.50E-03	-3.23E-02

Table S3. (Continued)

Precursor: Benzene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A^a	B^a	C^a	D^a
1VF	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
3VF	5.71E-05	-4.32E-03	1.02E-01	-5.19E-01
4VF	-1.07E-06	8.78E-05	-2.25E-03	2.02E-02
5VF	3.26E-07	-2.67E-05	6.82E-04	-2.98E-03
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	-2.69E-06	2.19E-04	-5.61E-03	4.95E-02
8VF	7.87E-07	-6.41E-05	1.66E-03	-1.15E-02
1F	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
3F	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
5F	-9.67E-07	8.06E-05	-2.11E-03	1.77E-02
6F	-8.63E-07	7.20E-05	-1.93E-03	1.96E-02
7F	1.07E-06	-8.82E-05	2.37E-03	-1.74E-02
8F	-1.32E-05	1.07E-03	-2.76E-02	2.30E-01
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-3.24E-07	2.64E-05	-6.82E-04	5.83E-03
5M	-1.31E-06	1.08E-04	-2.82E-03	2.46E-02
6M	-1.36E-05	1.11E-03	-2.84E-02	2.51E-01
7M	-7.75E-05	6.30E-03	-1.61E-01	1.31E+00
8M	1.68E-06	-1.37E-04	3.57E-03	-2.57E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-1.31E-04	1.07E-02	-2.79E-01	2.43E+00
5S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6S	4.01E-06	-3.31E-04	8.84E-03	-6.19E-02
7S	-6.73E-07	5.38E-05	-1.30E-03	2.34E-02
8S	5.18E-08	-4.64E-06	1.83E-04	-1.62E-03
1P	3.79E-05	-3.12E-03	8.12E-02	-5.58E-01
2P	1.81E-07	-1.34E-05	3.08E-04	-2.07E-03
3P	4.75E-06	-3.90E-04	1.04E-02	-7.69E-02
4P	3.20E-07	-1.59E-05	6.46E-06	1.28E-02
5P	1.13E-05	-9.20E-04	2.43E-02	-1.77E-01
6P	1.18E-05	-1.09E-03	3.69E-02	-1.58E-01
7P	8.12E-07	-4.52E-05	2.09E-04	1.45E-01
8P	1.68E-05	-1.38E-03	3.66E-02	-2.22E-01
1MA	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
3MA	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
5MA	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
7MA	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
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-2.67E-05	2.19E-03	-5.64E-02	5.36E-01

^a The stoichiometric coefficient is calculated by $\alpha = A \times (VOC:NO_x)^3 + B \times (VOC:NO_x)^2 + C \times (VOC:NO_x) + D$, where VOC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S3. (Continued)

Precursor: Toluene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	6.56E-08	-5.80E-06	1.32E-04	2.55E-05
6VF	4.61E-08	-4.93E-06	1.47E-04	-2.38E-04
7VF	3.61E-08	-2.90E-06	3.74E-05	1.10E-03
8VF	1.88E-07	-1.52E-05	2.36E-04	4.11E-03
1F	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
3F	8.88E-08	-7.81E-06	1.68E-04	6.68E-04
4F	1.28E-07	-1.22E-05	2.98E-04	5.14E-04
5F	1.70E-08	-1.29E-06	1.85E-05	3.70E-04
6F	1.47E-07	-9.19E-06	-4.99E-05	8.25E-03
7F	2.24E-07	-1.95E-05	3.93E-04	2.65E-03
8F	4.52E-08	-3.77E-06	5.56E-05	1.24E-03
1M	1.76E-08	-1.20E-06	3.07E-05	-1.24E-04
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-3.48E-06	3.14E-04	-8.77E-03	1.14E-01
4M	9.82E-09	9.69E-08	-6.48E-05	2.07E-03
5M	6.34E-08	-5.89E-06	1.02E-04	1.89E-03
6M	7.70E-08	-3.54E-06	-1.18E-04	5.69E-03
7M	3.03E-08	3.12E-07	-2.67E-04	1.33E-02
8M	8.86E-07	-7.53E-05	1.44E-03	1.12E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	-7.52E-07	8.28E-05	-1.29E-03	1.20E-02
4S	-8.08E-08	1.03E-05	-5.58E-04	1.29E-02
5S	7.47E-07	-5.73E-05	6.35E-04	2.71E-02
6S	7.83E-07	-5.13E-05	-2.31E-05	3.66E-02
7S	-4.98E-08	5.72E-06	-2.49E-04	4.60E-03
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-2.73E-06	2.84E-04	-1.01E-02	1.33E-01
2P	-7.61E-08	2.15E-05	-6.92E-04	1.46E-02
3P	6.32E-06	-6.36E-04	1.97E-02	-1.08E-01
4P	8.07E-07	-5.06E-05	-2.42E-04	5.27E-02
5P	7.42E-07	-3.22E-05	-1.86E-03	1.01E-01
6P	-1.50E-06	7.91E-05	3.18E-03	1.16E-01
7P	1.01E-06	-7.84E-05	4.73E-04	6.50E-02
8P	-5.81E-07	3.95E-05	-6.53E-05	3.04E-02
1MA	-1.09E-06	1.22E-04	-2.81E-04	2.18E-02
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	3.10E-07	-2.92E-05	5.43E-04	1.02E-02
GLY	1.81E-06	-1.67E-04	3.55E-03	4.04E-02

Table S3. (Continued)

Precursor: o-Xylene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	1.53E-07	-1.50E-05	4.65E-04	-3.86E-03
4VF	2.20E-07	-2.16E-05	6.57E-04	-5.23E-03
5VF	2.24E-07	-2.17E-05	6.76E-04	-5.52E-03
6VF	1.83E-07	-1.77E-05	5.24E-04	-3.94E-03
7VF	1.42E-06	-1.40E-04	4.39E-03	-3.58E-02
8VF	1.16E-06	-1.13E-04	3.63E-03	-3.07E-02
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	7.42E-07	-7.25E-05	2.24E-03	-1.84E-02
5F	1.14E-06	-1.13E-04	3.53E-03	-2.89E-02
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	5.07E-07	-5.07E-05	1.57E-03	-1.23E-02
8F	1.88E-07	-1.87E-05	5.84E-04	-4.77E-03
1M	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
3M	7.71E-07	-1.20E-04	5.21E-03	-2.80E-02
4M	1.35E-07	-1.37E-05	4.50E-04	-3.53E-03
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	1.65E-06	-1.66E-04	5.89E-03	-5.06E-02
7M	4.16E-06	-4.17E-04	1.37E-02	-1.13E-01
8M	7.34E-07	-7.27E-05	2.26E-03	-1.83E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	1.55E-08	-1.39E-06	4.41E-05	-3.76E-04
3S	-7.56E-07	7.34E-05	-2.24E-03	2.57E-02
4S	3.90E-07	-4.31E-05	1.61E-03	-1.24E-02
5S	7.33E-07	-6.92E-05	1.97E-03	-1.05E-02
6S	7.90E-07	-8.02E-05	2.62E-03	-1.60E-02
7S	1.35E-06	-1.34E-04	3.85E-03	-8.69E-03
8S	7.03E-06	-6.88E-04	2.01E-02	-5.20E-02
1P	7.15E-07	-1.06E-04	4.33E-03	-3.11E-02
2P	-3.75E-07	3.34E-05	-9.18E-04	1.31E-02
3P	9.95E-07	-2.38E-05	-2.84E-04	5.94E-02
4P	7.22E-07	-5.71E-05	3.18E-03	1.75E-02
5P	4.98E-06	-4.91E-04	1.47E-02	-7.80E-02
6P	3.60E-07	-6.84E-05	3.08E-03	2.56E-02
7P	3.56E-06	-3.95E-04	1.43E-02	-2.74E-02
8P	1.59E-06	-1.56E-04	5.21E-03	-4.52E-02
1MA	3.94E-08	-4.93E-06	4.40E-04	-4.18E-03
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	1.63E-06	-1.59E-04	4.76E-03	-3.63E-02
GLY	4.74E-06	-4.65E-04	1.40E-02	-1.05E-01

Table S3. (Continued)

Precursor: m-Xylene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-2.73E-09	3.43E-07	-1.12E-05	1.75E-04
5VF	-1.73E-08	1.98E-06	-5.64E-05	7.47E-04
6VF	-9.97E-09	1.15E-06	-4.25E-05	6.99E-04
7VF	-1.34E-07	1.77E-05	-5.61E-04	8.68E-03
8VF	-2.26E-07	3.43E-05	-1.06E-03	1.58E-02
1F	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
3F	-9.93E-09	7.38E-06	-2.97E-04	5.24E-03
4F	-1.52E-07	2.43E-05	-7.78E-04	1.23E-02
5F	-5.96E-09	8.85E-07	-2.80E-05	4.77E-04
6F	-3.97E-07	4.31E-05	-1.34E-03	2.01E-02
7F	-1.60E-07	2.89E-05	-7.64E-04	1.10E-02
8F	-8.96E-09	1.22E-06	-4.22E-05	6.71E-04
1M	-2.52E-09	3.49E-07	-7.32E-06	1.01E-04
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-1.22E-06	9.88E-05	-2.18E-03	3.21E-02
4M	-2.86E-08	4.79E-06	-1.68E-04	2.60E-03
5M	-3.32E-08	3.92E-06	-1.55E-04	2.27E-03
6M	-2.19E-08	3.67E-06	-1.59E-04	2.41E-03
7M	-1.23E-06	1.24E-04	-3.36E-03	5.79E-02
8M	-2.12E-08	2.93E-06	-1.02E-04	1.60E-03
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-2.43E-08	3.65E-06	-9.50E-05	8.69E-04
3S	3.51E-07	-4.03E-05	1.35E-03	-5.85E-03
4S	-3.43E-08	3.68E-06	-1.37E-04	3.18E-03
5S	-4.65E-08	2.81E-05	-1.75E-03	6.02E-02
6S	-6.52E-08	2.84E-05	-9.91E-04	1.57E-02
7S	3.08E-08	-5.92E-07	-1.77E-04	1.89E-02
8S	-1.43E-08	1.84E-06	-9.29E-05	1.95E-03
1P	-7.59E-07	5.91E-05	-1.24E-03	1.81E-02
2P	4.03E-07	-3.61E-05	1.25E-03	-5.79E-03
3P	-8.22E-07	1.48E-04	-6.39E-03	1.07E-01
4P	8.41E-07	-6.90E-05	1.55E-03	3.44E-02
5P	3.62E-07	-5.06E-05	1.62E-03	3.83E-02
6P	-3.51E-07	7.67E-06	1.86E-03	4.55E-02
7P	-2.09E-07	-2.40E-06	2.56E-03	1.09E-01
8P	1.10E-08	6.69E-07	-3.43E-05	6.24E-04
1MA	-1.20E-07	1.24E-05	-2.29E-04	2.23E-03
2MA	1.91E-08	-8.34E-07	1.29E-05	-1.05E-05
3MA	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
5MA	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
7MA	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
MGLY	-5.20E-07	6.44E-05	-2.34E-03	3.91E-02
GLY	-1.39E-07	1.84E-05	-7.74E-04	1.65E-02

Table S3. (Continued)

Precursor: p-Xylene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	7.91E-07	-9.87E-05	4.27E-03	-2.51E-02
8VF	1.58E-07	-1.83E-05	9.27E-04	-7.10E-03
1F	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
3F	5.08E-08	-5.29E-06	2.02E-04	-1.44E-03
4F	1.22E-07	-1.37E-05	5.06E-04	-3.19E-03
5F	1.93E-08	-1.91E-06	6.48E-05	-4.42E-04
6F	1.14E-07	-1.44E-05	5.93E-04	-2.71E-03
7F	3.24E-07	-3.49E-05	1.34E-03	-1.14E-02
8F	3.60E-08	-3.94E-06	1.42E-04	-8.67E-04
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-2.73E-07	2.09E-05	-2.37E-04	1.48E-02
5M	-3.25E-10	1.30E-08	-4.01E-07	1.72E-04
6M	1.11E-07	-1.33E-05	9.77E-04	-8.15E-03
7M	1.63E-06	-2.08E-04	8.91E-03	-5.32E-02
8M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-1.10E-08	6.77E-07	2.30E-05	-2.91E-04
3S	-4.05E-08	4.27E-06	-1.65E-04	2.91E-03
4S	2.94E-07	-3.37E-05	1.48E-03	-8.73E-03
5S	1.05E-06	-1.27E-04	4.53E-03	2.32E-02
6S	6.41E-08	-6.76E-06	3.32E-04	-2.42E-03
7S	1.89E-07	-1.80E-05	5.40E-04	-2.22E-03
8S	5.55E-07	-6.47E-05	3.28E-03	-2.57E-02
1P	4.28E-07	-4.22E-05	1.48E-03	-7.97E-03
2P	4.58E-08	-3.16E-06	1.56E-04	4.21E-04
3P	-6.19E-07	5.44E-05	-1.76E-03	6.51E-02
4P	2.85E-07	-2.66E-05	3.18E-03	-4.40E-03
5P	-2.12E-07	1.82E-06	2.76E-04	6.48E-02
6P	6.30E-07	-9.38E-05	4.43E-03	2.37E-02
7P	6.99E-08	5.16E-07	2.90E-04	9.86E-03
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	2.98E-08	-2.80E-06	1.24E-04	-9.56E-04
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	5.49E-07	-5.75E-05	1.87E-03	-4.23E-03
GLY	1.11E-06	-1.21E-04	4.26E-03	-1.94E-02

Table S3. (Continued)

Precursor: 123-TMB^a NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-4.28E-09	3.69E-07	-3.20E-06	1.72E-05
5VF	-1.49E-08	1.33E-06	-1.53E-05	9.26E-05
6VF	1.45E-09	-5.14E-07	3.83E-05	-1.70E-04
7VF	-2.11E-07	1.54E-05	6.03E-05	1.84E-03
8VF	-2.92E-09	6.01E-07	-3.97E-05	1.05E-03
1F	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
3F	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
5F	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
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-2.86E-07	1.90E-05	2.65E-04	-1.03E-03
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-3.83E-07	3.88E-05	-7.14E-04	4.64E-03
3M	-3.77E-08	4.79E-06	-2.56E-04	1.18E-02
4M	8.48E-07	-1.23E-04	6.18E-03	-1.37E-02
5M	4.75E-07	-4.30E-05	6.57E-04	2.99E-02
6M	-7.42E-07	7.86E-05	-1.64E-03	1.14E-02
7M	-5.71E-07	3.94E-05	6.44E-04	3.51E-03
8M	-6.98E-08	6.53E-06	-1.03E-04	6.73E-04
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	1.12E-07	-1.13E-05	3.08E-04	4.71E-03
4S	1.41E-08	-1.52E-06	4.04E-05	6.62E-04
5S	-1.97E-06	2.05E-04	-4.29E-03	4.11E-02
6S	-5.25E-07	4.30E-05	-2.50E-04	8.31E-04
7S	1.87E-07	-2.17E-05	6.62E-04	1.08E-02
8S	1.48E-06	-1.51E-04	3.69E-03	3.46E-01
1P	-3.51E-08	2.53E-06	2.09E-05	6.26E-04
2P	2.34E-07	-1.85E-05	2.47E-04	1.30E-02
3P	-5.00E-07	3.82E-05	2.48E-04	2.48E-02
4P	-6.79E-07	7.90E-05	-1.99E-03	3.48E-02
5P	3.21E-07	-2.29E-05	-3.29E-04	5.40E-02
6P	1.64E-07	-3.22E-05	2.24E-03	-2.28E-03
7P	2.33E-06	-2.89E-04	1.23E-02	-1.68E-02
8P	-2.15E-07	2.40E-05	-5.35E-04	3.81E-03
1MA	-5.77E-09	7.53E-07	-1.15E-05	9.99E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	7.95E-08	-1.72E-05	1.03E-03	4.51E-03
GLY	2.15E-08	-5.89E-06	4.22E-04	3.58E-03

^a “123-TMB” represents 1,2,3-trimethylbenzene.

Table S3. (Continued)

Precursor: 124-TMB^a NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	-1.61E-07	1.02E-05	-1.04E-06	2.17E-02
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-3.16E-08	4.68E-07	9.45E-05	5.97E-03
3F	-4.85E-08	5.70E-06	-2.64E-04	7.13E-03
4F	2.64E-07	-3.06E-05	9.98E-04	1.70E-02
5F	-3.98E-07	5.18E-05	-2.37E-03	5.29E-02
6F	-1.83E-07	8.95E-06	2.41E-05	2.55E-02
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-6.22E-10	8.53E-08	-1.55E-05	1.28E-03
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-8.16E-08	9.52E-06	-4.51E-04	1.53E-02
5M	-2.08E-08	1.09E-06	2.20E-05	2.84E-03
6M	-9.44E-08	1.15E-05	-5.09E-04	1.01E-02
7M	-3.65E-08	1.11E-05	-1.12E-03	1.36E-01
8M	-2.97E-10	-3.96E-08	-2.44E-05	3.09E-03
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-4.80E-10	4.14E-08	1.49E-06	9.38E-05
3S	-6.51E-09	1.20E-06	-6.80E-05	2.20E-03
4S	8.07E-08	-1.12E-05	5.69E-04	1.15E-02
5S	-3.57E-07	4.53E-05	-1.87E-03	9.22E-02
6S	-8.20E-08	9.39E-06	-4.01E-04	1.44E-02
7S	1.80E-08	2.60E-06	-4.32E-04	2.78E-02
8S	2.04E-07	-1.29E-05	-6.08E-04	1.92E-01
1P	-1.16E-08	5.95E-07	2.15E-05	8.45E-04
2P	1.78E-08	5.87E-07	-1.82E-04	7.98E-03
3P	5.72E-08	-7.43E-06	3.43E-04	3.03E-03
4P	-5.29E-07	2.57E-05	1.85E-03	5.49E-02
5P	5.78E-08	1.66E-06	-4.73E-04	2.98E-02
6P	7.43E-07	-8.00E-05	3.02E-03	3.88E-02
7P	-7.74E-08	5.57E-07	3.48E-04	5.60E-03
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	-1.42E-10	-1.20E-08	2.95E-06	1.92E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-3.30E-07	4.79E-05	-2.74E-03	8.26E-02
GLY	-5.17E-08	7.76E-06	-5.18E-04	2.07E-02

^a “124-TMB” represents 1,2,4-trimethylbenzene.

Table S3. (Continued)

Precursor: 135-TMB NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	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
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	1.30E-07	-1.52E-05	4.55E-04	1.19E-02
3F	-4.27E-08	5.28E-06	-2.42E-04	5.78E-03
4F	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
6F	-5.77E-07	5.90E-05	-1.83E-03	2.46E-02
7F	-8.60E-09	7.30E-07	-1.54E-05	1.12E-03
8F	-2.26E-07	2.10E-05	-4.00E-04	3.41E-02
1M	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
3M	-7.23E-09	7.07E-07	-2.02E-05	4.16E-04
4M	-6.70E-08	7.64E-06	-3.41E-04	1.09E-02
5M	9.17E-08	-9.40E-06	2.81E-04	-8.64E-04
6M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7M	-1.33E-07	3.00E-05	-2.97E-03	2.11E-01
8M	-5.78E-07	6.18E-05	-2.09E-03	2.80E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-1.39E-06	1.27E-04	-1.69E-03	8.25E-02
5S	6.99E-07	-7.07E-05	1.97E-03	2.40E-03
6S	2.76E-07	-3.28E-05	1.47E-03	1.58E-02
7S	2.47E-06	-2.40E-04	6.10E-03	1.67E-02
8S	4.75E-08	-3.74E-06	2.84E-05	2.51E-03
1P	-1.43E-07	1.40E-05	-2.24E-04	4.78E-03
2P	2.16E-07	-2.22E-05	6.70E-04	-3.28E-03
3P	4.82E-06	-5.08E-04	1.57E-02	-1.23E-02
4P	-3.44E-06	3.46E-04	-8.62E-03	1.26E-01
5P	4.46E-08	-4.57E-06	1.37E-04	-5.21E-04
6P	7.44E-06	-7.59E-04	2.25E-02	2.00E-02
7P	-3.78E-06	3.81E-04	-9.81E-03	9.36E-02
8P	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
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-3.93E-06	4.46E-04	-1.68E-02	2.59E-01
GLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00

^a “135-TMB” represents 1,3,5-trimethylbenzene.

Table S3. (Continued)

Precursor: Ethylbenzene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	-4.99E-08	3.88E-06	-9.41E-05	1.10E-03
6VF	-9.20E-08	6.90E-06	-1.62E-04	2.27E-03
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	-4.48E-07	3.33E-05	-7.21E-04	6.81E-03
1F	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
3F	-1.75E-07	1.09E-05	-1.56E-04	1.41E-03
4F	-3.52E-07	2.51E-05	-4.96E-04	4.46E-03
5F	-4.41E-08	3.20E-06	-6.21E-05	4.43E-04
6F	-3.07E-07	2.26E-05	-4.89E-04	5.60E-03
7F	-3.51E-07	2.70E-05	-6.53E-04	8.17E-03
8F	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
2M	-3.87E-08	2.22E-06	-9.42E-06	-7.51E-05
3M	3.85E-06	-2.69E-04	5.38E-03	-6.04E-03
4M	-5.08E-08	3.20E-06	-4.19E-05	4.01E-04
5M	-4.46E-08	2.93E-06	-5.17E-05	8.30E-04
6M	-4.27E-08	2.90E-06	-5.63E-05	7.56E-04
7M	-3.65E-07	2.94E-05	-7.00E-04	1.10E-02
8M	-1.44E-06	1.08E-04	-2.34E-03	3.34E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	1.69E-07	-9.87E-07	7.55E-06	2.18E-02
4S	-2.05E-06	1.48E-04	-3.19E-03	3.53E-02
5S	-1.25E-06	9.49E-05	-2.13E-03	2.11E-02
6S	-1.19E-07	9.00E-06	-2.09E-04	2.30E-03
7S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-1.08E-06	1.06E-04	-3.52E-03	4.59E-02
2P	1.01E-07	1.19E-06	-2.27E-04	1.24E-02
3P	6.92E-06	-6.29E-04	1.79E-02	-1.14E-01
4P	-1.69E-06	1.27E-04	-2.93E-03	3.56E-02
5P	-1.90E-06	2.60E-04	-1.06E-02	1.62E-01
6P	1.28E-06	-6.05E-05	3.80E-05	4.55E-02
7P	-7.61E-06	5.60E-04	-1.22E-02	2.79E-01
8P	-2.00E-05	1.79E-03	-5.70E-02	7.95E-01
1MA	1.11E-05	-7.75E-04	1.86E-02	-1.24E-01
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-3.20E-06	2.56E-04	-6.06E-03	7.22E-02

Table S3. (Continued)

Precursor: Propylbenzene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	-1.18E-07	1.07E-05	-2.71E-04	2.18E-03
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-1.99E-08	1.53E-06	-3.24E-05	7.66E-04
5VF	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
7VF	-6.70E-09	3.27E-07	7.22E-06	2.86E-04
8VF	-1.50E-07	1.38E-05	-3.79E-04	4.32E-03
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-8.75E-08	7.56E-06	-1.91E-04	1.76E-03
3F	-1.51E-07	1.34E-05	-3.43E-04	3.42E-03
4F	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
6F	-2.39E-07	1.95E-05	-4.70E-04	7.53E-03
7F	-2.43E-08	1.50E-06	-1.60E-05	9.67E-04
8F	3.48E-08	-3.13E-06	8.22E-05	-3.50E-04
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-3.66E-08	3.13E-06	-7.84E-05	6.62E-04
3M	5.65E-07	-5.74E-05	1.57E-03	1.06E-02
4M	-6.56E-08	5.62E-06	-1.41E-04	1.60E-03
5M	-2.17E-07	1.91E-05	-5.01E-04	4.54E-03
6M	-1.01E-07	8.55E-06	-2.06E-04	2.21E-03
7M	3.33E-07	-3.10E-05	8.74E-04	-5.20E-03
8M	-6.52E-07	5.55E-05	-1.28E-03	1.81E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-3.43E-08	3.17E-06	-8.64E-05	8.60E-04
3S	6.50E-07	-5.60E-05	1.56E-03	8.29E-03
4S	-2.43E-06	2.18E-04	-5.86E-03	6.15E-02
5S	-1.30E-06	1.16E-04	-3.10E-03	3.55E-02
6S	-3.37E-08	5.09E-06	-1.43E-04	1.18E-02
7S	-9.26E-07	7.66E-05	-1.86E-03	3.74E-02
8S	-3.60E-08	3.34E-06	-9.58E-05	9.60E-04
1P	-4.57E-07	4.64E-05	-1.75E-03	3.37E-02
2P	8.05E-07	-1.17E-04	5.22E-03	-2.90E-02
3P	-2.09E-06	1.81E-04	-4.64E-03	4.12E-02
4P	9.51E-06	-8.09E-04	1.95E-02	-9.88E-02
5P	6.82E-08	1.68E-06	-5.59E-04	2.30E-02
6P	-5.57E-07	4.40E-05	-1.20E-03	3.92E-02
7P	-1.67E-06	1.20E-04	-1.91E-03	1.82E-01
8P	-8.92E-06	9.34E-04	-3.48E-02	6.17E-01
1MA	4.83E-08	-1.79E-05	1.62E-03	-1.27E-02
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-2.67E-05	2.19E-03	-5.64E-02	5.36E-01

Table S3. (Continued)

Precursor: Terpene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	-1.25E-07	9.33E-06	-6.15E-05	2.75E-05
2VF	-1.63E-10	-1.74E-08	2.01E-06	-1.27E-05
3VF	7.41E-08	-6.44E-06	1.40E-04	-6.48E-05
4VF	-1.77E-09	4.96E-08	4.85E-06	-3.40E-05
5VF	6.08E-08	-7.17E-06	2.45E-04	5.53E-03
6VF	4.10E-09	-3.24E-07	4.87E-06	9.13E-05
7VF	9.10E-08	-7.97E-06	2.02E-04	6.39E-05
8VF	-1.20E-08	7.30E-07	2.30E-06	-2.69E-05
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-9.71E-09	1.04E-06	2.85E-06	8.45E-06
5F	-6.16E-08	4.90E-06	-4.75E-05	6.01E-04
6F	-2.29E-08	1.68E-06	-1.05E-05	4.15E-04
7F	1.86E-07	-1.49E-05	1.53E-04	1.38E-02
8F	1.32E-09	-6.58E-08	3.68E-06	6.51E-05
1M	-7.28E-07	6.14E-05	-7.32E-04	2.44E-03
2M	3.02E-07	-2.90E-05	8.51E-04	-2.53E-03
3M	-8.02E-07	6.28E-05	-4.52E-04	4.82E-04
4M	-1.77E-06	1.34E-04	-5.57E-04	4.20E-02
5M	1.79E-06	-1.83E-04	5.50E-03	3.51E-02
6M	1.37E-06	-8.33E-05	-1.90E-03	4.68E-01
7M	8.67E-07	-6.62E-05	6.31E-04	6.38E-02
8M	-3.68E-08	2.72E-06	-1.12E-05	-2.19E-05
1S	-2.33E-07	8.99E-06	6.79E-04	2.84E-03

Lumped Species	A	B	C	D
2S	2.27E-07	-2.50E-05	1.04E-03	3.71E-03
3S	1.06E-06	-1.08E-04	3.33E-03	6.34E-03
4S	4.62E-06	-4.27E-04	1.11E-02	4.03E-02
5S	2.30E-06	-1.93E-04	3.71E-03	4.09E-02
6S	-1.08E-06	7.90E-05	-4.63E-04	9.47E-03
7S	-9.86E-08	6.17E-06	-8.14E-06	1.55E-03
8S	-1.66E-10	-1.20E-09	1.23E-06	-7.86E-06
1P	-2.22E-07	1.67E-05	-1.15E-04	2.47E-03
2P	6.43E-07	-6.84E-05	2.28E-03	-6.95E-03
3P	-3.70E-08	2.34E-06	2.02E-05	-2.10E-04
4P	-5.36E-07	4.61E-05	-7.33E-04	1.19E-02
5P	-1.48E-06	1.24E-04	-2.36E-03	1.59E-01
6P	2.78E-08	-2.34E-06	4.13E-05	9.63E-04
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8P	1.77E-06	-1.54E-04	3.40E-03	3.69E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	4.84E-09	-1.65E-07	-2.14E-05	1.46E-03
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	-3.10E-09	1.24E-07	8.61E-06	-5.64E-05
5MA	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
7MA	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
MGLY	-2.92E-08	3.52E-06	-1.50E-04	2.57E-03
GLY	3.72E-08	-3.37E-06	8.99E-05	-2.77E-05

Table S3. (Continued)

Precursor: Isoprene NO_x level: Low NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	2.09E-10	-1.91E-08	5.24E-07	-3.41E-06
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	2.25E-13	-2.09E-11	5.96E-10	-4.21E-09
7VF	1.04E-06	-9.24E-05	2.29E-03	-4.93E-03
8VF	2.09E-08	-1.86E-06	4.60E-05	-2.82E-05
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	3.52E-08	-3.41E-06	1.05E-04	-3.05E-04
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	-1.34E-07	1.62E-05	-6.64E-04	9.79E-03
7F	2.74E-07	-2.68E-05	8.42E-04	-2.77E-03
8F	-1.37E-08	1.08E-06	-2.17E-05	2.49E-04
1M	7.04E-09	-6.53E-07	1.90E-05	-1.12E-04
2M	2.25E-08	-2.14E-06	6.03E-05	-1.43E-04
3M	2.95E-07	-2.74E-05	7.58E-04	-3.44E-04
4M	3.76E-10	-1.81E-08	-4.36E-07	3.07E-05
5M	8.14E-08	-7.57E-06	2.23E-04	-1.42E-06
6M	-1.37E-07	4.34E-06	6.14E-04	6.92E-03
7M	-6.86E-07	5.46E-05	-1.07E-03	1.49E-02
8M	2.46E-07	1.37E-05	-2.83E-03	1.43E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-1.06E-13	1.14E-11	-3.93E-10	4.48E-09
3S	-8.40E-11	1.18E-08	-5.54E-07	9.49E-06
4S	5.61E-09	8.12E-08	-3.91E-05	1.14E-03
5S	3.36E-08	-2.88E-06	7.96E-05	1.56E-03
6S	5.06E-07	-4.39E-05	1.17E-03	1.74E-02
7S	2.27E-09	3.09E-06	-2.64E-04	8.49E-03
8S	5.91E-07	-5.41E-05	1.49E-03	1.14E-02
1P	1.89E-07	-1.79E-05	5.09E-04	-1.12E-03
2P	2.67E-07	-2.27E-05	4.74E-04	4.87E-03
3P	3.14E-08	-2.85E-06	7.30E-05	-1.80E-04
4P	-2.55E-08	2.09E-06	-4.22E-05	5.23E-04
5P	-1.21E-08	1.69E-06	-8.72E-05	1.90E-03
6P	-4.49E-07	4.52E-05	-1.45E-03	2.07E-02
7P	-2.08E-06	1.66E-04	-2.65E-03	3.47E-02
8P	-7.89E-07	1.06E-04	-4.70E-03	9.99E-02
1MA	6.47E-09	-6.00E-07	1.61E-05	-2.39E-05
2MA	1.03E-08	-9.70E-07	2.77E-05	-1.08E-04
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	-4.67E-10	3.86E-08	-6.91E-07	4.62E-06
5MA	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
7MA	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
MGLY	-1.35E-07	1.74E-05	-8.43E-04	2.14E-02
GLY	-4.19E-08	6.53E-06	-3.99E-04	1.23E-02
IEPOX	1.59E-06	-1.60E-04	5.50E-03	-3.23E-02

Table S3. (Continued)

Precursor: Benzene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A^a	B^a	C^a	D^a
1VF	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
3VF	2.23E-04	-3.09E-03	1.31E-02	-1.63E-02
4VF	2.51E-04	-6.48E-03	4.84E-02	-4.35E-02
5VF	2.66E-06	-3.74E-05	1.64E-04	-2.05E-04
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	6.02E-04	-1.48E-02	1.09E-01	-1.47E-01
8VF	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
2F	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
4F	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
6F	7.97E-07	-1.13E-05	4.80E-05	-6.15E-05
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	7.44E-04	-1.71E-02	1.23E-01	-1.62E-01
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	6.41E-06	-1.00E-04	5.80E-04	-7.11E-04
5M	8.22E-07	-1.15E-05	4.88E-05	-6.09E-05
6M	3.51E-05	-5.01E-04	2.50E-03	-1.07E-03
7M	1.52E-06	-2.13E-05	9.05E-05	-1.07E-04
8M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	3.67E-06	-5.22E-05	2.21E-04	-2.86E-04
5S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6S	2.20E-05	-3.15E-04	1.90E-03	-1.13E-03
7S	1.42E-05	-2.02E-04	1.01E-03	-9.95E-04
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6P	1.67E-04	-2.43E-03	1.37E-02	-1.13E-02
7P	1.69E-04	-3.59E-03	2.42E-02	1.25E-02
8P	3.50E-03	-8.73E-02	6.43E-01	-5.39E-01
1MA	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
3MA	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
5MA	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
7MA	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
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	1.26E-03	-2.93E-02	2.10E-01	-2.24E-01

^a The stoichiometric coefficient is calculated by $\alpha = A \times (VOC:NO_x)^3 + B \times (VOC:NO_x)^2 + C \times (VOC:NO_x) + D$, where VOC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S3. (Continued)

Precursor: Toluene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	1.62E-06	-4.68E-05	4.69E-04	-5.96E-04
3VF	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
5VF	2.16E-06	-5.93E-05	4.76E-04	-4.10E-04
6VF	8.65E-07	-2.49E-05	2.19E-04	-2.97E-04
7VF	9.18E-06	-2.88E-04	3.15E-03	1.05E-03
8VF	-1.86E-05	5.31E-04	-4.92E-03	3.35E-02
1F	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
3F	3.74E-06	-1.18E-04	1.34E-03	7.14E-04
4F	2.23E-06	-6.57E-05	6.38E-04	-6.77E-04
5F	4.41E-08	-7.66E-07	5.46E-06	-7.44E-06
6F	1.55E-05	-4.49E-04	4.26E-03	-3.70E-03
7F	-3.95E-05	8.74E-04	-2.66E-03	6.00E-02
8F	-7.90E-05	1.96E-03	-1.04E-02	5.77E-02
1M	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
3M	2.06E-05	-5.58E-04	4.75E-03	-6.31E-03
4M	-9.51E-07	-2.00E-05	1.61E-03	6.16E-03
5M	2.68E-06	-1.06E-04	2.17E-03	-1.09E-03
6M	2.85E-06	-2.18E-04	6.27E-03	1.54E-02
7M	7.04E-05	-1.80E-03	1.24E-02	4.89E-02
8M	-7.18E-05	1.84E-03	-1.21E-02	1.08E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	4.63E-09	-5.69E-08	2.34E-07	-2.88E-07
3S	1.74E-09	-1.94E-08	8.19E-08	-1.04E-07
4S	3.80E-06	-1.24E-04	1.55E-03	-2.15E-03
5S	1.80E-05	-4.73E-04	3.70E-03	2.73E-02
6S	4.54E-05	-1.32E-03	1.43E-02	1.33E-02
7S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	3.11E-08	-4.50E-07	1.92E-06	-2.38E-06
2P	1.21E-07	-1.62E-06	6.81E-06	-8.41E-06
3P	2.13E-04	-5.80E-03	4.80E-02	-3.49E-02
4P	-1.59E-04	4.39E-03	-3.64E-02	1.52E-01
5P	1.22E-04	-3.47E-03	3.17E-02	-4.53E-03
6P	8.74E-05	-2.08E-03	8.39E-03	1.15E-01
7P	-2.16E-04	5.94E-03	-5.11E-02	2.72E-01
8P	-2.82E-04	7.84E-03	-6.75E-02	3.07E-01
1MA	2.71E-08	-3.24E-07	1.33E-06	-1.65E-06
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-8.10E-05	1.72E-03	-2.19E-03	6.24E-02
GLY	-4.17E-06	-2.72E-04	1.01E-02	1.73E-01

Table S3. (Continued)

Precursor: o-Xylene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	-2.51E-07	-1.81E-05	5.91E-04	-7.13E-04
3VF	6.02E-06	-1.85E-04	1.73E-03	4.70E-03
4VF	2.30E-06	-6.69E-05	5.70E-04	-2.61E-05
5VF	2.09E-06	-5.12E-05	2.09E-04	4.01E-03
6VF	3.80E-06	-1.02E-04	7.30E-04	4.41E-04
7VF	-4.22E-05	8.64E-04	1.72E-03	1.06E-01
8VF	-1.69E-05	5.15E-04	-5.57E-03	4.66E-02
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-1.59E-05	1.76E-04	3.62E-03	-5.33E-03
5F	4.51E-06	-1.76E-04	2.11E-03	-2.53E-03
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	1.46E-05	-4.38E-04	3.94E-03	9.73E-03
8F	-3.43E-06	3.26E-05	1.62E-03	9.90E-03
1M	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
3M	1.34E-05	-3.45E-04	2.28E-03	1.18E-03
4M	3.35E-09	1.98E-08	1.12E-07	-3.22E-07
5M	2.47E-07	-3.93E-05	8.48E-04	-1.13E-03
6M	-5.80E-06	-1.64E-05	3.26E-03	-4.25E-03
7M	-1.46E-06	6.87E-05	-1.67E-03	1.04E-01
8M	6.72E-06	-3.28E-04	6.71E-03	2.59E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	5.03E-10	1.13E-08	-2.11E-08	-8.98E-10
3S	7.33E-11	4.08E-09	2.19E-08	-5.89E-08
4S	7.14E-11	1.56E-09	1.98E-08	-2.94E-08
5S	-2.10E-06	3.37E-05	-8.66E-05	3.00E-02
6S	-6.92E-06	-5.54E-05	4.93E-03	3.87E-03
7S	2.09E-05	-5.50E-04	3.70E-03	1.11E-02
8S	3.49E-05	-9.57E-04	7.48E-03	1.33E-01
1P	1.67E-10	1.43E-10	6.66E-09	-1.76E-08
2P	3.93E-09	8.04E-09	3.99E-08	-1.33E-07
3P	8.24E-05	-2.17E-03	1.43E-02	5.91E-02
4P	-4.79E-05	1.26E-03	-7.76E-03	7.89E-02
5P	1.70E-05	-6.31E-04	7.05E-03	3.41E-02
6P	4.47E-06	-7.88E-05	-3.42E-04	2.12E-02
7P	-3.92E-05	1.43E-03	-1.79E-02	2.44E-01
8P	-7.62E-05	2.08E-03	-1.58E-02	1.44E-01
1MA	2.93E-10	5.86E-09	9.16E-08	-2.11E-07
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	3.45E-05	-1.29E-03	1.78E-02	3.31E-02
GLY	5.01E-05	-1.48E-03	1.32E-02	4.06E-02

Table S3. (Continued)

Precursor: m-Xylene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	-2.76E-08	-3.92E-07	2.48E-07	4.34E-04
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	-8.42E-07	-6.33E-06	5.46E-04	2.29E-02
8VF	-1.49E-05	4.55E-04	-4.48E-03	4.79E-02
1F	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
3F	-1.35E-07	-2.26E-05	6.54E-04	2.07E-02
4F	-6.70E-07	1.23E-05	-2.00E-05	2.39E-03
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	-6.33E-07	8.40E-06	4.33E-04	-2.39E-04
7F	9.44E-05	-2.59E-03	2.19E-02	1.88E-01
8F	2.69E-05	-8.83E-04	9.87E-03	1.49E-02
1M	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
3M	-3.97E-07	1.04E-05	-7.22E-05	8.38E-04
4M	-1.84E-06	3.57E-05	2.20E-03	-2.11E-03
5M	1.64E-08	-8.71E-07	1.84E-05	-7.27E-06
6M	1.04E-07	-6.73E-06	1.06E-03	-9.49E-04
7M	-1.37E-05	4.27E-04	-4.44E-03	8.53E-02
8M	4.33E-05	-1.38E-03	1.45E-02	3.42E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-1.41E-07	2.77E-06	3.35E-05	-2.12E-05
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5S	-4.87E-06	1.17E-04	-3.06E-04	2.69E-02
6S	5.49E-07	-7.00E-06	2.62E-03	2.27E-02
7S	-1.22E-06	3.09E-05	-1.97E-04	6.55E-03
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	6.15E-10	-9.68E-09	4.37E-08	-5.70E-08
2P	6.04E-08	-8.52E-07	3.78E-06	-4.84E-06
3P	-9.42E-06	2.55E-04	-1.76E-03	2.94E-02
4P	1.97E-05	-4.75E-04	3.15E-03	8.65E-02
5P	-3.47E-06	9.53E-05	-6.38E-04	3.04E-02
6P	-1.42E-05	4.88E-04	-6.76E-03	6.49E-02
7P	2.34E-06	2.64E-04	-8.91E-03	3.44E-01
8P	-1.10E-05	3.92E-04	-4.74E-03	2.95E-02
1MA	1.41E-09	-1.89E-08	8.28E-08	-1.05E-07
2MA	2.68E-09	-3.85E-08	1.69E-07	-2.15E-07
3MA	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
5MA	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
7MA	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
MGLY	8.67E-05	-2.95E-03	3.40E-02	1.09E-01
GLY	1.14E-05	-3.61E-04	3.76E-03	4.57E-02

Table S3. (Continued)

Precursor: p-Xylene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	4.87E-05	-1.59E-03	1.38E-02	6.44E-02
8VF	-6.04E-06	2.13E-04	-2.43E-03	2.87E-02
1F	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
3F	1.53E-06	-1.04E-04	1.45E-03	3.73E-03
4F	-8.19E-06	1.77E-04	-3.87E-04	1.78E-03
5F	-7.38E-07	2.01E-05	-1.07E-04	1.49E-04
6F	1.58E-05	-7.07E-04	8.84E-03	-1.14E-02
7F	1.34E-05	-3.30E-04	1.59E-03	2.16E-02
8F	1.01E-05	-2.75E-04	1.88E-03	3.72E-03
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	9.00E-05	-2.87E-03	2.76E-02	-3.29E-02
5M	7.71E-07	-2.65E-05	2.85E-04	-3.78E-04
6M	5.75E-05	-1.63E-03	1.39E-02	-7.54E-03
7M	2.26E-05	-9.41E-04	1.06E-02	7.99E-02
8M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	2.47E-06	-8.57E-05	8.96E-04	-1.13E-03
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-2.59E-05	6.85E-04	-3.59E-03	4.98E-03
5S	-5.66E-05	-1.83E-04	2.22E-02	-5.40E-03
6S	3.07E-05	-1.04E-03	1.04E-02	-8.12E-03
7S	2.73E-05	-7.69E-04	6.34E-03	-7.86E-03
8S	-2.56E-05	1.09E-03	-1.65E-02	1.74E-01
1P	-1.00E-05	2.83E-04	-1.50E-03	2.09E-03
2P	-5.55E-06	1.53E-04	-8.06E-04	1.12E-03
3P	-1.13E-04	3.44E-03	-3.22E-02	1.13E-01
4P	-5.74E-05	1.89E-03	-1.49E-02	7.37E-02
5P	4.06E-05	-1.68E-03	2.06E-02	1.31E-02
6P	-2.36E-05	8.50E-04	-8.04E-03	7.08E-02
7P	-9.44E-05	2.96E-03	-3.01E-02	1.38E-01
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	-5.93E-07	1.85E-05	-9.65E-05	1.32E-04
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	9.30E-05	-2.98E-03	2.66E-02	1.62E-02
GLY	3.12E-05	-1.26E-03	1.32E-02	7.57E-02

Table S3. (Continued)

Precursor: 123-TMB^a NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	-3.21E-08	7.66E-07	-1.81E-06	-7.37E-08
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	5.21E-05	-1.52E-03	1.26E-02	1.49E-04
8VF	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
2F	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
4F	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
6F	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
8F	7.12E-05	-2.09E-03	1.74E-02	-2.22E-03
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-3.98E-07	9.95E-06	-1.12E-05	-3.39E-05
3M	2.33E-05	-6.77E-04	5.57E-03	-2.25E-03
4M	6.76E-07	-2.06E-05	2.13E-04	-3.24E-04
5M	4.14E-05	-1.21E-03	1.03E-02	-1.64E-02
6M	-3.11E-04	8.97E-03	-7.36E-02	3.31E-01
7M	8.70E-05	-2.71E-03	2.46E-02	8.83E-02
8M	-1.78E-04	5.13E-03	-3.96E-02	1.41E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	1.23E-05	-3.65E-04	3.17E-03	-5.62E-03
4S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5S	1.23E-04	-3.71E-03	3.29E-02	-9.08E-03
6S	1.37E-04	-4.30E-03	4.12E-02	-3.83E-02
7S	4.08E-05	-1.19E-03	9.88E-03	-9.22E-03
8S	9.14E-05	-2.74E-03	2.33E-02	2.54E-01
1P	-7.28E-08	1.90E-06	-2.34E-06	-6.40E-06
2P	2.51E-05	-7.05E-04	5.65E-03	-1.27E-03
3P	2.43E-07	-9.24E-06	1.53E-04	-2.88E-04
4P	-2.20E-04	6.33E-03	-5.11E-02	2.36E-01
5P	2.63E-04	-7.71E-03	6.55E-02	-9.79E-02
6P	-6.86E-05	2.11E-03	-2.01E-02	8.73E-02
7P	-1.31E-04	4.00E-03	-3.82E-02	2.07E-01
8P	-1.95E-04	5.67E-03	-4.76E-02	2.07E-01
1MA	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
3MA	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
5MA	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
7MA	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
MGLY	-2.90E-05	6.39E-04	-1.90E-03	8.04E-02
GLY	1.22E-05	-4.49E-04	5.15E-03	2.66E-02

^a “123-TMB” represents 1,2,3-trimethylbenzene.

Table S3. (Continued)

Precursor: 124-TMB^a NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	2.28E-05	-4.47E-04	2.29E-03	2.99E-02
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	3.69E-07	-6.47E-06	3.29E-05	-4.78E-05
3F	7.00E-06	-1.74E-04	1.50E-03	1.89E-04
4F	7.48E-07	-1.65E-05	1.25E-04	-1.47E-04
5F	9.76E-06	-2.04E-04	1.52E-03	-2.00E-03
6F	-5.82E-05	1.24E-03	-1.07E-02	3.41E-01
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-2.41E-06	-3.87E-06	7.69E-04	1.23E-02
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	2.80E-05	-6.33E-04	5.72E-03	-5.94E-03
5M	7.93E-06	-1.69E-04	1.24E-03	2.62E-04
6M	8.95E-06	-2.01E-04	1.69E-03	-1.26E-03
7M	8.02E-05	-1.89E-03	1.49E-02	5.75E-02
8M	-8.88E-06	4.54E-05	1.55E-03	3.56E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	2.56E-07	-4.83E-06	2.85E-05	-4.09E-05
4S	2.31E-07	-4.07E-06	2.07E-05	-3.01E-05
5S	3.62E-05	-8.68E-04	7.18E-03	1.98E-03
6S	2.89E-05	-6.88E-04	6.06E-03	-1.75E-03
7S	1.22E-05	-2.95E-04	2.45E-03	2.30E-04
8S	1.94E-05	-3.23E-04	-1.44E-03	2.94E-01
1P	6.92E-08	-1.23E-06	6.26E-06	-9.11E-06
2P	3.49E-06	-7.58E-05	5.86E-04	-5.51E-04
3P	7.77E-08	-1.37E-06	6.99E-06	-1.02E-05
4P	-2.10E-05	6.08E-04	-7.33E-03	1.83E-01
5P	6.02E-06	-1.35E-04	1.01E-03	1.12E-03
6P	-1.67E-05	4.69E-04	-6.02E-03	8.57E-02
7P	-6.79E-06	2.52E-04	-4.82E-03	1.71E-01
8P	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
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	4.11E-05	-1.36E-03	1.58E-02	1.08E-01
GLY	8.20E-06	-2.11E-04	1.83E-03	2.59E-02

^a "124-TMB" represents 1,2,4-trimethylbenzene.

Table S3. (Continued)

Precursor: 135-TMB NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	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
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	1.96E-07	-3.20E-06	1.61E-05	-2.32E-05
3F	2.18E-06	-6.01E-05	4.57E-04	2.33E-03
4F	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
6F	-2.16E-05	3.34E-04	2.04E-03	9.78E-02
7F	3.32E-08	-5.44E-07	2.72E-06	-3.92E-06
8F	-3.24E-06	1.50E-04	-2.44E-03	3.25E-02
1M	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
3M	5.80E-09	-9.46E-08	4.74E-07	-6.83E-07
4M	2.31E-07	-3.33E-06	2.10E-05	-3.04E-05
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7M	1.72E-05	-3.96E-04	1.38E-03	7.10E-02
8M	-5.48E-06	-3.87E-04	1.26E-02	1.30E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	1.23E-05	-3.12E-04	1.73E-03	4.03E-02
5S	1.61E-07	-2.66E-06	1.61E-05	-2.29E-05
6S	5.72E-06	-1.29E-04	7.35E-04	8.79E-03
7S	9.54E-06	-2.60E-04	1.92E-03	9.37E-03
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	7.08E-08	-1.18E-06	5.92E-06	-8.53E-06
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	1.77E-07	-2.91E-06	1.46E-05	-2.11E-05
4P	-5.62E-05	1.40E-03	-8.37E-03	1.81E-01
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6P	-2.02E-05	7.25E-04	-9.42E-03	1.27E-01
7P	-8.32E-05	2.29E-03	-1.93E-02	3.57E-01
8P	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
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	7.67E-05	-2.79E-03	3.32E-02	2.70E-01
GLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00

^a “135-TMB” represents 1,3,5-trimethylbenzene.

Table S3. (Continued)

Precursor: Ethylbenzene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	-4.50E-09	4.70E-07	-2.24E-06	3.00E-06
2VF	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
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	1.86E-06	-4.96E-05	4.01E-04	1.44E-04
6VF	2.50E-06	-1.15E-04	1.57E-03	3.58E-03
7VF	1.25E-08	-1.70E-07	6.87E-07	-8.11E-07
8VF	1.27E-06	-4.10E-05	3.41E-04	1.22E-02
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	4.92E-06	-1.84E-04	2.20E-03	3.23E-03
3F	1.31E-06	-1.73E-05	6.96E-05	-8.21E-05
4F	4.73E-06	-1.27E-04	1.14E-03	-3.47E-04
5F	2.01E-07	-3.30E-06	2.14E-05	-2.99E-05
6F	-3.06E-05	5.17E-04	-4.87E-04	3.12E-02
7F	1.95E-05	-1.02E-03	1.55E-02	4.79E-03
8F	-3.37E-05	5.67E-04	1.68E-04	7.59E-03
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	5.26E-08	-7.11E-07	2.88E-06	-3.42E-06
3M	3.97E-05	-9.86E-04	7.68E-03	-7.02E-03
4M	6.52E-07	-6.12E-06	2.13E-05	-2.22E-05
5M	8.13E-07	-1.56E-05	8.23E-05	2.33E-04
6M	5.85E-08	5.53E-06	-2.96E-05	4.24E-05
7M	2.00E-06	-2.26E-04	4.07E-03	3.54E-02
8M	-2.04E-04	3.25E-03	7.39E-03	4.27E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	7.56E-06	-1.92E-04	2.03E-03	2.11E-02
5S	2.14E-05	-5.27E-04	4.54E-03	2.64E-03
6S	4.68E-06	-1.31E-04	1.13E-03	2.91E-03
7S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	1.32E-06	-1.83E-05	7.50E-05	-8.95E-05
2P	2.39E-06	-5.03E-05	3.46E-04	-2.78E-04
3P	1.23E-04	-3.35E-03	2.76E-02	2.26E-02
4P	-3.38E-05	8.27E-04	-5.01E-03	5.36E-02
5P	8.31E-06	-2.07E-04	1.84E-03	2.11E-02
6P	4.17E-06	-1.13E-04	1.06E-03	6.75E-03
7P	2.36E-05	-1.02E-03	7.86E-03	3.30E-01
8P	3.44E-04	-8.88E-03	6.82E-02	5.16E-02
1MA	4.73E-07	-6.44E-06	2.63E-05	-3.13E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	4.58E-05	-2.34E-03	3.53E-02	5.79E-02

Table S3. (Continued)

Precursor: Propylbenzene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	1.30E-09	-2.00E-08	8.59E-08	-1.06E-07
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-1.79E-06	3.82E-05	-1.10E-04	1.65E-04
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	-2.14E-06	3.30E-05	1.34E-04	4.48E-04
7VF	-7.59E-07	1.94E-05	-8.62E-05	1.11E-04
8VF	2.18E-06	-8.18E-05	7.56E-04	3.94E-03
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-3.83E-06	7.14E-05	1.18E-05	5.95E-04
3F	-1.72E-06	3.89E-05	-1.23E-04	1.80E-04
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	4.84E-08	-7.17E-07	3.04E-06	-3.71E-06
6F	-5.52E-05	1.02E-03	1.28E-05	3.21E-02
7F	-3.33E-05	7.07E-04	-1.51E-03	4.62E-03
8F	-1.44E-05	3.22E-04	-3.87E-04	7.32E-03
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	2.51E-08	-3.71E-07	1.57E-06	-1.91E-06
3M	-1.93E-05	4.64E-04	-2.00E-03	2.58E-03
4M	6.42E-07	-8.66E-06	3.55E-05	-4.18E-05
5M	2.09E-07	-3.82E-06	5.06E-05	1.15E-05
6M	7.21E-07	-9.95E-06	4.12E-05	-4.82E-05
7M	-4.22E-05	1.02E-03	-2.10E-03	1.65E-02
8M	-8.27E-05	2.14E-03	-5.33E-03	3.05E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	2.87E-08	-4.03E-07	1.67E-06	-2.01E-06
3S	-8.42E-08	2.18E-06	-9.38E-06	1.37E-05
4S	-1.05E-05	7.74E-05	2.64E-03	3.93E-03
5S	-1.62E-05	3.41E-04	-5.58E-04	2.94E-03
6S	-6.17E-06	1.11E-04	3.76E-06	8.43E-04
7S	-2.84E-05	4.47E-04	1.19E-03	1.74E-02
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	6.80E-07	-1.01E-05	4.28E-05	-5.24E-05
2P	-1.31E-04	2.64E-03	-5.91E-03	1.16E-02
3P	1.57E-05	-4.94E-04	4.56E-03	3.43E-02
4P	1.32E-05	-4.15E-04	3.63E-03	1.48E-03
5P	-5.01E-07	1.23E-05	-5.85E-05	7.56E-05
6P	-3.24E-06	-5.34E-04	1.11E-02	7.16E-02
7P	-1.16E-04	1.19E-03	1.39E-02	1.10E-01
8P	-9.12E-05	1.67E-03	-2.22E-03	4.38E-02
1MA	2.04E-07	-3.01E-06	1.27E-05	-1.55E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-1.46E-04	2.93E-03	-3.23E-03	5.64E-02
GLY	1.26E-03	-2.93E-02	2.10E-01	-2.24E-01

Table S3. (Continued)

Precursor: Terpene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	4.54E-07	-3.76E-06	1.11E-05	-1.07E-05
2VF	9.53E-09	-7.37E-08	2.03E-07	-1.86E-07
3VF	-1.58E-06	2.59E-05	-1.34E-05	-3.67E-05
4VF	3.16E-08	-2.47E-07	6.85E-07	-6.34E-07
5VF	2.05E-05	-4.49E-04	3.34E-03	-1.61E-03
6VF	-7.64E-08	1.23E-06	1.69E-07	7.17E-05
7VF	-3.09E-06	5.57E-05	-9.87E-05	5.75E-05
8VF	2.47E-08	3.57E-07	-7.02E-07	3.70E-07
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-9.84E-08	3.00E-06	-6.66E-06	3.86E-06
5F	1.99E-06	-4.07E-05	2.77E-04	-1.34E-04
6F	1.60E-06	-3.36E-05	2.31E-04	-1.07E-04
7F	1.20E-06	-5.55E-05	7.13E-04	1.14E-02
8F	-2.29E-07	5.60E-06	-3.76E-05	1.49E-04
1M	1.51E-06	-1.27E-05	3.75E-05	-3.63E-05
2M	-2.99E-06	4.52E-05	2.18E-04	-4.94E-04
3M	2.91E-06	-2.23E-05	6.12E-05	-5.62E-05
4M	6.65E-05	-1.38E-03	9.94E-03	1.97E-02
5M	7.81E-05	-1.87E-03	1.73E-02	8.97E-03
6M	1.39E-04	-4.40E-03	4.04E-02	3.39E-01
7M	1.72E-05	-3.94E-04	3.23E-03	5.54E-02
8M	1.87E-07	-1.29E-06	3.38E-06	-3.04E-06
1S	1.24E-05	-2.93E-04	2.99E-03	-2.77E-03

Lumped Species	A	B	C	D
2S	7.51E-06	-2.20E-04	2.91E-03	-2.41E-03
3S	-1.26E-06	1.53E-05	1.82E-03	1.14E-02
4S	-9.68E-05	1.71E-03	-1.12E-03	5.39E-02
5S	-4.49E-05	6.73E-04	6.14E-04	3.52E-02
6S	1.14E-05	-1.51E-04	2.78E-04	1.17E-02
7S	-4.74E-07	3.23E-05	-4.26E-04	3.36E-03
8S	5.90E-09	-3.34E-08	7.73E-08	-6.38E-08
1P	6.93E-07	-5.17E-06	2.48E-05	2.28E-03
2P	-5.35E-06	8.83E-05	7.29E-04	-1.48E-03
3P	1.90E-07	-3.70E-07	5.77E-07	-3.12E-07
4P	1.30E-05	-2.51E-04	1.36E-03	7.18E-03
5P	-6.92E-05	1.98E-03	-2.07E-02	2.21E-01
6P	-1.52E-06	3.20E-05	-1.92E-04	1.43E-03
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8P	-2.82E-05	3.46E-04	2.32E-03	-3.75E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	-1.26E-06	3.03E-05	-2.61E-04	2.08E-03
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	2.12E-08	2.22E-07	-1.21E-06	1.46E-06
5MA	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
7MA	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
MGLY	2.95E-06	-6.47E-05	3.63E-04	1.29E-03
GLY	-9.14E-07	1.67E-05	-1.14E-05	-8.02E-06

Table S3. (Continued)

Precursor: Isoprene NO_x level: High NO_x Aging stats: Fresh				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-8.65E-10	2.31E-08	-1.12E-07	1.60E-07
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	-3.53E-13	1.31E-11	-7.56E-11	1.14E-10
7VF	1.47E-05	-4.09E-04	4.08E-03	-3.57E-03
8VF	1.12E-06	-2.89E-05	2.34E-04	-2.85E-04
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-2.13E-07	5.89E-06	-1.27E-05	2.21E-04
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	2.45E-05	-6.59E-04	5.10E-03	-4.88E-03
7F	-8.48E-06	2.17E-04	-1.21E-03	2.12E-03
8F	-2.46E-07	6.52E-06	-3.89E-05	5.74E-05
1M	-1.28E-08	4.80E-07	-1.70E-06	1.12E-05
2M	2.98E-07	-7.11E-06	7.26E-05	-5.07E-05
3M	-5.55E-06	1.35E-04	-6.30E-04	3.27E-03
4M	1.87E-07	-4.75E-06	3.32E-05	-1.51E-05
5M	-4.34E-06	1.05E-04	-5.60E-04	9.19E-04
6M	-2.34E-05	6.07E-04	-3.52E-03	1.00E-02
7M	2.09E-06	-3.76E-05	6.44E-04	2.05E-03
8M	-9.84E-05	2.15E-03	-1.46E-02	1.49E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	3.49E-10	-8.48E-09	5.62E-08	-5.84E-08
3S	7.75E-08	-1.85E-06	1.08E-05	6.84E-06
4S	3.50E-06	-9.47E-05	7.72E-04	-9.58E-04
5S	2.10E-07	-6.33E-06	6.85E-05	1.91E-03
6S	-7.48E-06	1.51E-04	-2.50E-05	1.79E-02
7S	-1.54E-05	3.25E-04	-1.48E-03	3.57E-03
8S	-2.09E-05	4.61E-04	-1.18E-03	6.83E-03
1P	-3.30E-06	8.06E-05	-3.14E-04	6.88E-04
2P	-2.96E-07	-5.70E-06	2.28E-04	6.57E-03
3P	-3.30E-07	7.42E-06	-1.78E-05	7.57E-05
4P	-8.51E-07	2.12E-05	-1.31E-04	2.50E-04
5P	-4.46E-06	1.03E-04	-5.82E-04	8.63E-04
6P	7.32E-05	-1.85E-03	1.27E-02	-3.79E-03
7P	-4.84E-05	1.26E-03	-7.51E-03	1.47E-02
8P	-6.78E-06	-3.55E-04	9.27E-03	1.01E-02
1MA	-1.60E-07	3.77E-06	-1.60E-05	2.42E-05
2MA	-1.67E-07	4.18E-06	-1.95E-05	2.87E-05
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	2.44E-10	8.36E-09	-7.88E-08	1.33E-07
5MA	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
7MA	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
MGLY	-1.06E-05	1.74E-04	-2.42E-05	7.27E-03
GLY	1.80E-06	-7.68E-05	9.30E-04	5.12E-03
IEPOX	-1.99E-05	6.00E-04	-3.61E-03	5.38E-03

Table S3. (Continued)

Precursor: Benzene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A^a	B^a	C^a	D^a
1VF	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
3VF	3.29E-04	8.05E-03	4.03E-03	-2.10E-02
4VF	-1.66E-05	3.57E-03	-2.54E-02	8.02E-02
5VF	-1.23E-06	-3.76E-05	2.48E-04	-2.98E-04
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	-4.91E-06	2.03E-03	-1.21E-02	4.11E-02
8VF	1.89E-06	-1.81E-05	6.69E-05	-7.06E-05
1F	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
3F	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
5F	-9.13E-06	-8.72E-05	3.21E-04	-3.33E-04
6F	-1.50E-05	-1.75E-04	6.69E-04	-7.17E-04
7F	4.51E-06	-1.10E-06	4.09E-06	-4.32E-06
8F	2.35E-06	2.15E-03	-6.82E-03	4.36E-02
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	9.22E-07	2.14E-06	2.66E-04	-6.43E-05
5M	-1.40E-05	-1.39E-04	5.20E-04	-5.45E-04
6M	-1.07E-04	-1.23E-03	7.56E-03	-5.36E-03
7M	-6.21E-04	-5.52E-03	2.05E-02	-2.17E-02
8M	6.31E-06	-2.79E-06	1.03E-05	-1.09E-05
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-1.39E-03	-1.39E-02	5.18E-02	-5.51E-02
5S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6S	5.27E-05	-4.93E-04	4.99E-03	1.69E-04
7S	-3.18E-06	-1.00E-04	2.39E-03	-2.07E-03
8S	6.31E-07	-3.94E-08	1.47E-07	-1.55E-07
1P	8.01E-05	-1.05E-03	3.88E-03	-4.10E-03
2P	2.65E-07	-2.16E-07	8.00E-07	-8.45E-07
3P	1.97E-05	-2.31E-06	8.55E-06	-9.02E-06
4P	-2.52E-05	-3.74E-04	1.42E-03	-1.51E-03
5P	4.36E-05	-3.21E-05	1.19E-04	-1.25E-04
6P	8.20E-05	-5.01E-03	4.08E-02	-2.24E-02
7P	-5.44E-05	3.08E-03	-1.18E-02	1.03E-01
8P	6.42E-04	4.98E-02	-3.00E-01	1.11E+00
1MA	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
3MA	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
5MA	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
7MA	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
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-1.09E-04	8.03E-03	-4.01E-02	1.77E-01

^a The stoichiometric coefficient is calculated by $\alpha = A \times (VOC:NO_x)^3 + B \times (VOC:NO_x)^2 + C \times (VOC:NO_x) + D$, where VOC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S3. (Continued)

Precursor: Toluene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	-6.21E-06	1.66E-04	-1.28E-03	3.33E-03
6VF	-1.54E-06	4.26E-05	-3.15E-04	1.27E-03
7VF	-1.71E-05	4.83E-04	-4.24E-03	1.27E-02
8VF	-3.37E-05	9.15E-04	-7.47E-03	2.26E-02
1F	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
3F	-5.26E-06	1.42E-04	-1.12E-03	4.09E-03
4F	-3.08E-08	-1.33E-05	3.65E-04	2.39E-04
5F	2.06E-06	-5.15E-05	3.70E-04	-2.98E-04
6F	2.48E-05	-6.31E-04	4.40E-03	-1.55E-05
7F	-9.10E-05	2.54E-03	-2.16E-02	5.97E-02
8F	-4.76E-05	1.32E-03	-1.12E-02	3.02E-02
1M	-1.49E-07	3.54E-06	-1.27E-05	1.18E-05
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	2.43E-04	-6.27E-03	4.45E-02	-1.57E-02
4M	7.06E-06	-1.36E-04	2.61E-04	4.88E-03
5M	1.20E-05	-2.81E-04	1.64E-03	1.67E-03
6M	1.16E-05	-1.64E-04	-9.58E-04	1.73E-02
7M	-2.12E-04	5.93E-03	-5.08E-02	1.39E-01
8M	-1.46E-04	4.02E-03	-3.36E-02	1.01E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	-6.22E-06	1.28E-04	5.66E-05	-7.55E-04
4S	8.66E-05	-2.30E-03	1.74E-02	-2.33E-02
5S	1.57E-04	-4.06E-03	2.93E-02	-1.99E-02
6S	-5.62E-05	1.42E-03	-1.05E-02	4.99E-02
7S	-3.30E-06	4.11E-05	2.79E-04	-7.97E-04
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-1.72E-04	3.62E-03	-1.53E-02	1.80E-02
2P	-5.13E-06	-1.86E-06	1.98E-03	-4.33E-03
3P	-2.48E-04	7.77E-03	-7.29E-02	2.39E-01
4P	-6.13E-05	1.13E-03	-2.39E-03	2.11E-02
5P	6.59E-04	-1.69E-02	1.17E-01	-7.36E-02
6P	9.31E-05	-1.92E-03	7.98E-03	1.83E-01
7P	-4.34E-04	1.09E-02	-7.54E-02	1.68E-01
8P	-3.37E-04	8.75E-03	-6.45E-02	1.49E-01
1MA	-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
3MA	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
5MA	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
7MA	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
MGLY	-5.53E-05	1.57E-03	-1.39E-02	5.12E-02
GLY	-2.58E-04	7.38E-03	-6.54E-02	2.42E-01

Table S3. (Continued)

Precursor: o-Xylene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	-6.42E-06	1.79E-04	-1.50E-03	3.79E-03
4VF	-8.50E-07	2.32E-05	-1.82E-04	6.95E-04
5VF	-7.01E-07	1.83E-05	-1.27E-04	4.45E-04
6VF	-5.35E-07	1.11E-05	-3.68E-05	2.51E-04
7VF	-2.68E-05	7.36E-04	-6.00E-03	1.59E-02
8VF	-2.06E-05	5.69E-04	-4.70E-03	1.22E-02
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-2.91E-05	8.21E-04	-7.06E-03	1.89E-02
5F	-4.75E-05	1.41E-03	-1.31E-02	3.94E-02
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-9.13E-06	2.48E-04	-1.96E-03	5.14E-03
8F	-3.15E-06	8.72E-05	-7.20E-04	1.91E-03
1M	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
3M	-1.75E-04	4.97E-03	-4.34E-02	1.38E-01
4M	-3.79E-07	1.03E-05	-5.13E-05	1.96E-04
5M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6M	-3.48E-05	9.80E-04	-8.13E-03	2.13E-02
7M	-8.75E-05	2.43E-03	-1.99E-02	5.32E-02
8M	-9.72E-06	2.70E-04	-2.22E-03	6.18E-03
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	1.51E-08	-3.92E-07	3.57E-06	-8.34E-07
3S	8.16E-06	-2.48E-04	2.68E-03	-4.74E-03
4S	1.16E-07	-1.01E-05	3.42E-04	-4.84E-04
5S	-7.92E-06	2.69E-04	-3.21E-03	1.95E-02
6S	-4.26E-05	1.14E-03	-8.97E-03	2.58E-02
7S	-6.00E-05	1.66E-03	-1.41E-02	5.85E-02
8S	-6.27E-05	1.46E-03	-9.52E-03	1.33E-01
1P	-2.02E-06	4.09E-05	7.05E-04	-1.46E-03
2P	6.45E-06	-1.94E-04	2.12E-03	-3.58E-03
3P	1.56E-04	-4.08E-03	2.74E-02	4.18E-02
4P	3.97E-05	-1.38E-03	1.72E-02	-2.73E-02
5P	-2.67E-04	7.44E-03	-6.14E-02	1.80E-01
6P	1.87E-05	-4.83E-04	3.90E-03	4.47E-02
7P	-2.03E-04	5.65E-03	-4.39E-02	1.70E-01
8P	-1.76E-05	4.83E-04	-3.88E-03	9.79E-03
1MA	-3.30E-07	1.23E-05	-2.75E-05	1.67E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-2.32E-05	6.42E-04	-5.44E-03	1.78E-02
GLY	-7.37E-05	2.04E-03	-1.70E-02	5.46E-02

Table S3. (Continued)

Precursor: m-Xylene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	4.11E-07	-1.11E-05	8.95E-05	-1.43E-04
5VF	1.69E-06	-4.43E-05	3.43E-04	-4.84E-04
6VF	1.96E-06	-5.38E-05	4.38E-04	-6.98E-04
7VF	2.21E-06	-2.34E-05	-3.08E-04	6.35E-03
8VF	1.06E-05	-2.53E-04	1.74E-03	2.26E-03
1F	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
3F	4.42E-06	-9.11E-05	3.36E-04	3.18E-03
4F	1.67E-05	-4.25E-04	3.19E-03	-2.16E-03
5F	8.59E-07	-2.30E-05	1.90E-04	-2.95E-04
6F	2.03E-05	-4.72E-04	2.38E-03	1.13E-02
7F	5.82E-06	-1.21E-04	7.55E-04	2.02E-03
8F	4.85E-07	-1.04E-05	4.42E-05	3.52E-04
1M	3.95E-08	-8.54E-07	9.37E-06	-1.77E-05
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-3.61E-05	1.16E-03	-1.24E-02	6.17E-02
4M	-7.58E-08	2.04E-05	-4.71E-04	3.78E-03
5M	-4.10E-06	1.17E-04	-1.10E-03	4.52E-03
6M	5.87E-06	-1.43E-04	8.05E-04	1.41E-03
7M	-1.88E-05	7.19E-04	-8.13E-03	5.42E-02
8M	1.49E-06	-3.31E-05	1.56E-04	8.23E-04
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	2.79E-07	-5.60E-06	2.61E-05	1.16E-04
3S	-5.85E-07	-2.12E-05	9.96E-04	-1.72E-03
4S	8.61E-06	-2.42E-04	2.05E-03	-3.10E-03
5S	8.50E-05	-1.66E-03	1.61E-03	1.10E-01
6S	1.23E-05	-2.79E-04	1.61E-03	4.76E-03
7S	5.35E-05	-1.48E-03	1.21E-02	-9.70E-03
8S	5.98E-06	-1.49E-04	9.09E-04	9.55E-04
1P	-7.32E-06	1.61E-04	-6.68E-05	-3.17E-04
2P	5.43E-06	-1.49E-04	1.62E-03	-2.53E-03
3P	-1.21E-05	4.07E-04	-7.18E-03	9.83E-02
4P	1.36E-05	-6.83E-04	1.15E-02	-1.93E-02
5P	5.84E-05	-1.39E-03	9.42E-03	3.04E-02
6P	-7.04E-05	2.11E-03	-1.71E-02	8.97E-02
7P	-7.94E-05	2.35E-03	-1.69E-02	1.36E-01
8P	3.22E-07	-6.42E-06	3.03E-05	2.08E-04
1MA	-3.38E-07	1.29E-05	-3.87E-05	3.54E-05
2MA	1.31E-07	-3.32E-06	2.75E-05	-4.53E-05
3MA	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
5MA	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
7MA	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
MGLY	8.61E-05	-2.25E-03	1.65E-02	-1.19E-02
GLY	2.85E-05	-7.23E-04	4.80E-03	4.56E-03

Table S3. (Continued)

Precursor: p-Xylene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	-1.43E-04	4.08E-03	-3.41E-02	9.30E-02
8VF	-1.60E-05	4.61E-04	-3.79E-03	1.02E-02
1F	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
3F	-9.00E-06	2.58E-04	-2.19E-03	5.67E-03
4F	-3.99E-06	1.18E-04	-9.99E-04	3.53E-03
5F	1.92E-07	-5.17E-06	4.86E-05	-4.82E-05
6F	-4.04E-05	1.17E-03	-1.02E-02	2.86E-02
7F	-1.29E-05	3.56E-04	-2.85E-03	7.57E-03
8F	-3.58E-06	1.02E-04	-8.52E-04	2.33E-03
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-7.70E-05	2.23E-03	-1.97E-02	6.66E-02
5M	-1.83E-06	5.30E-05	-4.74E-04	1.49E-03
6M	-2.52E-05	7.29E-04	-6.11E-03	1.61E-02
7M	-2.14E-04	6.10E-03	-5.01E-02	1.37E-01
8M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-7.65E-07	2.26E-05	-1.90E-04	4.97E-04
3S	2.04E-06	-6.80E-05	7.32E-04	-1.26E-03
4S	1.20E-05	-3.36E-04	3.06E-03	-3.93E-03
5S	-3.99E-04	1.16E-02	-1.02E-01	3.21E-01
6S	-2.88E-05	8.24E-04	-7.06E-03	1.83E-02
7S	7.40E-06	-1.97E-04	1.54E-03	-1.05E-03
8S	-7.28E-05	2.09E-03	-1.75E-02	4.64E-02
1P	6.41E-06	-1.86E-04	1.96E-03	-3.00E-03
2P	2.99E-06	-8.95E-05	9.08E-04	-1.32E-03
3P	1.72E-05	-5.32E-04	4.65E-03	4.14E-02
4P	-2.26E-06	-1.67E-05	3.26E-03	4.96E-04
5P	-2.45E-05	7.09E-04	-6.70E-03	9.17E-02
6P	-8.25E-05	2.27E-03	-1.65E-02	8.47E-02
7P	2.66E-05	-8.19E-04	8.04E-03	-1.15E-02
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	-1.67E-07	5.03E-06	-1.49E-05	1.78E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-5.03E-05	1.48E-03	-1.32E-02	4.66E-02
GLY	-1.08E-04	3.10E-03	-2.62E-02	8.01E-02

Table S3. (Continued)

Precursor: 123-TMB^a NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	1.28E-07	-4.45E-06	4.55E-05	-8.25E-05
5VF	7.38E-07	-2.29E-05	2.09E-04	-3.67E-04
6VF	7.56E-07	-2.83E-05	3.11E-04	-6.09E-04
7VF	-6.26E-05	1.94E-03	-1.95E-02	6.88E-02
8VF	1.55E-07	-9.73E-06	1.77E-04	-3.98E-04
1F	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
3F	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
5F	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
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-7.95E-05	2.49E-03	-2.54E-02	9.19E-02
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	6.36E-06	-2.01E-04	1.89E-03	-3.22E-03
3M	4.79E-06	-8.83E-05	-4.87E-04	2.00E-02
4M	-1.49E-05	2.58E-05	7.45E-03	-1.74E-02
5M	1.86E-04	-5.04E-03	3.85E-02	-2.89E-02
6M	-1.34E-04	4.01E-03	-3.77E-02	1.11E-01
7M	-2.51E-04	7.52E-03	-7.09E-02	2.27E-01
8M	-2.49E-05	7.56E-04	-7.24E-03	2.19E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	-1.70E-05	5.39E-04	-5.24E-03	2.14E-02
4S	4.09E-06	-1.08E-04	7.65E-04	2.46E-04
5S	5.05E-05	-9.35E-04	-1.47E-03	8.12E-02
6S	-6.87E-05	2.23E-03	-2.39E-02	9.10E-02
7S	-1.03E-05	3.93E-04	-5.58E-03	4.57E-02
8S	7.87E-05	-2.74E-03	2.86E-02	2.94E-01
1P	2.85E-08	-4.68E-06	1.81E-04	-3.78E-04
2P	1.83E-05	-5.93E-04	6.27E-03	-8.27E-03
3P	1.51E-05	-6.86E-04	1.03E-02	-1.66E-02
4P	-9.10E-05	2.67E-03	-2.37E-02	7.95E-02
5P	4.84E-04	-1.19E-02	6.93E-02	7.32E-02
6P	-4.52E-05	1.28E-03	-1.06E-02	4.60E-02
7P	-1.81E-04	5.09E-03	-3.74E-02	1.28E-01
8P	-6.39E-05	1.88E-03	-1.73E-02	4.82E-02
1MA	-5.37E-09	2.33E-07	3.33E-06	-7.39E-06
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-3.00E-05	9.36E-04	-1.07E-02	6.44E-02
GLY	-2.85E-05	9.23E-04	-1.01E-02	4.72E-02

^a “123-TMB” represents 1,2,3-trimethylbenzene.

Table S3. (Continued)

Precursor: 124-TMB^a NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	-6.89E-05	1.80E-03	-1.17E-02	2.36E-02
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-1.64E-05	4.17E-04	-2.40E-03	3.98E-03
3F	-1.94E-05	5.04E-04	-3.53E-03	8.44E-03
4F	-5.21E-05	1.27E-03	-6.73E-03	1.35E-02
5F	-1.71E-04	4.69E-03	-3.87E-02	1.21E-01
6F	-7.21E-05	1.89E-03	-1.21E-02	2.33E-02
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-3.14E-06	8.05E-05	-5.06E-04	1.00E-03
1M	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
3M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4M	-4.27E-05	1.08E-03	-7.11E-03	1.50E-02
5M	-8.98E-06	2.37E-04	-1.55E-03	3.24E-03
6M	-3.28E-05	8.49E-04	-6.12E-03	1.44E-02
7M	-4.08E-04	1.05E-02	-7.03E-02	1.73E-01
8M	-7.82E-06	2.02E-04	-1.27E-03	2.49E-03
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-2.58E-07	6.69E-06	-3.89E-05	6.17E-05
3S	-2.09E-06	5.93E-05	-5.84E-04	3.75E-03
4S	-2.61E-05	6.12E-04	-2.52E-03	4.37E-03
5S	-3.07E-04	8.61E-03	-7.30E-02	2.52E-01
6S	-4.48E-05	1.15E-03	-7.90E-03	1.81E-02
7S	-2.63E-05	6.36E-04	-4.25E-03	2.92E-02
8S	-7.24E-05	1.37E-03	-1.74E-03	1.36E-01
1P	-4.59E-07	9.77E-06	4.49E-05	-3.85E-05
2P	1.74E-05	-4.52E-04	2.68E-03	8.87E-03
3P	-1.08E-05	2.67E-04	-1.29E-03	1.93E-03
4P	-1.50E-04	3.86E-03	-2.13E-02	3.75E-02
5P	4.97E-05	-1.24E-03	6.18E-03	4.27E-02
6P	-5.59E-05	1.42E-03	-8.83E-03	6.58E-02
7P	-1.87E-05	5.11E-04	-3.14E-03	5.62E-03
8P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1MA	-7.77E-08	2.11E-06	-1.16E-05	1.82E-05
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-1.42E-04	3.49E-03	-2.18E-02	6.16E-02
GLY	-4.10E-05	1.02E-03	-6.37E-03	1.73E-02

^a “124-TMB” represents 1,2,4-trimethylbenzene.

Table S3. (Continued)

Precursor: 135-TMB NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	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
7VF	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
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-2.69E-06	-4.66E-05	2.66E-03	-5.16E-03
3F	6.22E-07	-2.71E-05	2.39E-04	3.61E-03
4F	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
6F	-1.32E-05	2.58E-04	-9.02E-04	7.34E-03
7F	-6.35E-07	7.99E-06	9.86E-05	-1.76E-04
8F	-1.47E-05	3.23E-04	-1.24E-03	2.64E-02
1M	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
3M	-2.06E-07	3.04E-06	1.83E-05	-3.50E-05
4M	9.54E-08	-8.83E-05	2.00E-03	-3.47E-03
5M	3.17E-06	-9.15E-05	8.49E-04	-1.20E-03
6M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7M	-1.64E-04	4.51E-03	-4.05E-02	3.10E-01
8M	-6.48E-06	8.91E-05	-1.90E-04	1.26E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-4.02E-05	6.48E-04	3.94E-03	8.01E-03
5S	2.68E-05	-8.37E-04	8.60E-03	-1.21E-02
6S	-7.18E-06	6.27E-05	2.08E-03	9.13E-03
7S	1.20E-04	-3.45E-03	3.05E-02	-1.81E-02
8S	2.97E-06	-6.58E-05	1.70E-04	4.65E-03
1P	-4.08E-06	8.65E-05	-1.36E-04	1.27E-04
2P	5.57E-06	-1.57E-04	1.44E-03	-2.40E-03
3P	6.74E-05	-2.55E-03	3.54E-02	-6.05E-02
4P	-7.72E-05	1.72E-03	-7.23E-03	4.06E-02
5P	1.33E-06	-3.85E-05	3.58E-04	-4.91E-04
6P	5.35E-05	-1.25E-03	9.45E-03	1.71E-01
7P	-5.03E-05	1.37E-03	-1.11E-02	4.60E-02
8P	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
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	7.16E-05	-2.37E-03	1.67E-02	1.38E-01
GLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00

^a “135-TMB” represents 1,3,5-trimethylbenzene.

Table S3. (Continued)

Precursor: Ethylbenzene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	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
5VF	-5.03E-06	1.29E-04	-9.39E-04	2.03E-03
6VF	-1.73E-05	4.54E-04	-3.51E-03	8.31E-03
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	-1.43E-05	3.89E-04	-3.21E-03	9.66E-03
1F	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
3F	5.37E-06	-1.37E-04	1.06E-03	-1.60E-03
4F	1.05E-06	-1.70E-05	2.65E-05	1.63E-03
5F	-1.46E-06	3.98E-05	-3.46E-04	1.09E-03
6F	-2.46E-05	6.54E-04	-5.20E-03	1.37E-02
7F	-1.30E-04	3.43E-03	-2.73E-02	6.65E-02
8F	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
2M	2.00E-07	-6.58E-06	7.13E-05	-1.26E-04
3M	-3.36E-04	9.02E-03	-7.42E-02	2.12E-01
4M	5.10E-06	-1.27E-04	8.99E-04	-1.26E-03
5M	8.22E-07	-2.02E-05	1.77E-04	-1.86E-04
6M	1.99E-06	-5.03E-05	3.89E-04	-5.71E-04
7M	-1.13E-04	2.99E-03	-2.37E-02	5.90E-02
8M	-8.48E-05	2.40E-03	-2.09E-02	7.15E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	-5.28E-05	9.70E-04	-1.78E-03	-2.95E-04
4S	1.20E-04	-2.48E-03	1.04E-02	3.17E-02
5S	-1.77E-05	6.15E-04	-6.97E-03	3.22E-02
6S	-9.83E-06	2.51E-04	-1.82E-03	3.89E-03
7S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8S	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1P	-4.47E-05	7.90E-04	-1.37E-03	-5.31E-05
2P	3.35E-04	-8.08E-03	5.25E-02	-5.06E-02
3P	1.19E-04	-2.60E-03	1.68E-02	-1.36E-02
4P	1.23E-04	-3.28E-03	2.53E-02	-3.18E-02
5P	-2.05E-04	4.75E-03	-2.68E-02	6.16E-02
6P	3.55E-05	-1.35E-03	1.54E-02	-1.11E-02
7P	-1.78E-04	4.08E-03	-2.15E-02	1.81E-01
8P	1.25E-03	-3.34E-02	2.51E-01	-7.60E-02
1MA	-1.52E-05	4.22E-04	-2.07E-03	2.65E-03
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-1.35E-04	3.93E-03	-3.56E-02	1.27E-01

Table S3. (Continued)

Precursor: Propylbenzene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	-8.40E-07	1.84E-05	-9.05E-05	1.19E-04
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-1.84E-06	5.68E-05	-5.39E-04	2.04E-03
5VF	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
7VF	1.26E-06	-2.49E-05	1.18E-04	2.18E-04
8VF	-6.68E-06	1.65E-04	-1.31E-03	5.68E-03
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	-1.28E-06	3.25E-05	-3.33E-04	2.10E-03
3F	-3.47E-06	7.01E-05	-3.20E-04	1.04E-03
4F	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
6F	3.57E-05	-6.55E-04	6.49E-04	2.61E-02
7F	1.45E-05	-2.79E-04	5.97E-04	7.65E-03
8F	5.11E-06	-8.91E-05	9.58E-06	3.68E-03
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-2.75E-07	5.99E-06	-2.69E-05	3.28E-05
3M	2.80E-04	-7.52E-03	5.70E-02	-6.60E-02
4M	-3.11E-06	6.57E-05	-2.99E-04	3.74E-04
5M	-6.81E-06	1.45E-04	-7.49E-04	1.25E-03
6M	-3.07E-06	6.46E-05	-2.75E-04	3.23E-04
7M	3.01E-05	-6.07E-04	2.17E-03	8.41E-03
8M	2.32E-05	-5.58E-04	2.94E-03	1.40E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	-2.23E-06	4.55E-05	-2.09E-04	2.62E-04
3S	9.13E-06	-1.46E-04	2.06E-03	-3.88E-03
4S	6.32E-05	-2.35E-03	2.37E-02	-2.91E-02
5S	6.13E-05	-1.70E-03	1.35E-02	-1.16E-02
6S	-2.04E-05	5.90E-04	-4.26E-03	1.08E-02
7S	3.60E-06	-1.47E-04	1.02E-03	2.87E-02
8S	-3.16E-06	6.46E-05	-3.05E-04	3.89E-04
1P	-6.62E-05	1.46E-03	-6.91E-03	8.79E-03
2P	-3.02E-04	8.06E-03	-6.51E-02	1.81E-01
3P	-9.36E-05	1.98E-03	-1.12E-02	3.12E-02
4P	-9.30E-05	2.41E-03	-1.41E-02	2.36E-02
5P	-8.35E-06	-5.39E-05	4.02E-03	-7.51E-03
6P	-2.19E-04	5.66E-03	-4.29E-02	1.21E-01
7P	-2.34E-04	6.12E-03	-4.50E-02	2.46E-01
8P	-1.42E-04	-2.52E-03	8.99E-02	-9.21E-02
1MA	5.56E-06	-5.78E-05	2.05E-04	-2.30E-04
2MA	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
4MA	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
6MA	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
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-1.14E-07	2.99E-06	-1.48E-05	1.92E-05
GLY	1.46E-04	-3.38E-03	1.82E-02	3.62E-02

Table S3. (Continued)

Precursor: Terpene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	4.83E-07	-4.29E-06	1.39E-05	-1.44E-05
2VF	1.05E-08	-9.08E-08	2.93E-07	-3.05E-07
3VF	-3.29E-07	2.89E-06	1.08E-04	-1.97E-04
4VF	3.47E-08	-3.03E-07	9.80E-07	-1.02E-06
5VF	2.28E-05	-4.91E-04	3.56E-03	-1.90E-03
6VF	3.53E-07	-6.68E-06	4.18E-05	1.67E-05
7VF	-4.40E-07	6.92E-06	1.58E-04	-2.82E-04
8VF	7.14E-08	-5.01E-07	3.81E-06	-5.60E-06
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	2.18E-08	7.95E-07	4.97E-06	-1.15E-05
5F	1.88E-06	-3.88E-05	2.67E-04	-1.21E-04
6F	1.56E-06	-3.27E-05	2.27E-04	-1.01E-04
7F	-7.74E-07	-1.92E-05	5.22E-04	1.17E-02
8F	2.25E-07	-2.77E-06	6.41E-06	9.13E-05
1M	1.60E-06	-1.44E-05	4.64E-05	-4.81E-05
2M	-2.63E-06	3.86E-05	2.53E-04	-5.40E-04
3M	3.12E-06	-2.63E-05	8.21E-05	-8.38E-05
4M	4.82E-05	-1.04E-03	8.16E-03	2.21E-02
5M	1.10E-04	-2.46E-03	2.04E-02	4.86E-03
6M	-2.63E-04	3.01E-03	1.42E-03	3.91E-01
7M	4.81E-05	-9.64E-04	6.22E-03	5.14E-02
8M	2.13E-07	-1.76E-06	5.89E-06	-6.36E-06
1S	2.20E-05	-4.70E-04	3.92E-03	-4.00E-03

Lumped Species	A	B	C	D
2S	2.10E-05	-4.68E-04	4.21E-03	-4.14E-03
3S	1.59E-05	-3.00E-04	3.48E-03	9.24E-03
4S	4.85E-05	-9.65E-04	1.29E-02	3.53E-02
5S	5.00E-05	-1.07E-03	9.80E-03	2.30E-02
6S	-2.78E-05	5.69E-04	-3.51E-03	1.67E-02
7S	-2.25E-06	6.49E-05	-5.98E-04	3.58E-03
8S	6.72E-09	-4.84E-08	1.56E-07	-1.68E-07
1P	-4.43E-07	1.57E-05	-8.52E-05	2.43E-03
2P	-2.60E-06	3.79E-05	9.94E-04	-1.83E-03
3P	2.70E-07	-1.84E-06	8.30E-06	-1.05E-05
4P	4.91E-06	-1.03E-04	5.75E-04	8.21E-03
5P	-2.43E-04	5.17E-03	-3.75E-02	2.43E-01
6P	-1.40E-06	2.98E-05	-1.81E-04	1.42E-03
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8P	1.68E-05	-4.82E-04	6.68E-03	-9.52E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	-7.55E-07	2.10E-05	-2.12E-04	2.01E-03
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	2.76E-08	1.05E-07	-5.95E-07	6.39E-07
5MA	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
7MA	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
MGLY	3.64E-06	-7.73E-05	4.30E-04	1.20E-03
GLY	3.91E-07	-7.34E-06	1.15E-04	-1.75E-04

Table S3. (Continued)

Precursor: Isoprene NO_x level: High NO_x Aging stats: Aged				
Lumped Species	A	B	C	D
1VF	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
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-8.65E-10	2.31E-08	-1.12E-07	1.60E-07
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	-3.53E-13	1.31E-11	-7.56E-11	1.14E-10
7VF	1.47E-05	-4.09E-04	4.08E-03	-3.57E-03
8VF	1.12E-06	-2.89E-05	2.34E-04	-2.85E-04
1F	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
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-2.13E-07	5.89E-06	-1.27E-05	2.21E-04
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	2.45E-05	-6.59E-04	5.10E-03	-4.88E-03
7F	-8.48E-06	2.17E-04	-1.21E-03	2.12E-03
8F	-2.46E-07	6.52E-06	-3.89E-05	5.74E-05
1M	-1.28E-08	4.80E-07	-1.70E-06	1.12E-05
2M	2.98E-07	-7.11E-06	7.26E-05	-5.07E-05
3M	-5.55E-06	1.35E-04	-6.30E-04	3.27E-03
4M	1.87E-07	-4.75E-06	3.32E-05	-1.51E-05
5M	-4.34E-06	1.05E-04	-5.60E-04	9.19E-04
6M	-2.34E-05	6.07E-04	-3.52E-03	1.00E-02
7M	2.09E-06	-3.76E-05	6.44E-04	2.05E-03
8M	-9.84E-05	2.15E-03	-1.46E-02	1.49E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Lumped Species	A	B	C	D
2S	3.49E-10	-8.48E-09	5.62E-08	-5.84E-08
3S	7.75E-08	-1.85E-06	1.08E-05	6.84E-06
4S	3.50E-06	-9.47E-05	7.72E-04	-9.58E-04
5S	2.10E-07	-6.33E-06	6.85E-05	1.91E-03
6S	-7.48E-06	1.51E-04	-2.50E-05	1.79E-02
7S	-1.54E-05	3.25E-04	-1.48E-03	3.57E-03
8S	-2.09E-05	4.61E-04	-1.18E-03	6.83E-03
1P	-3.30E-06	8.06E-05	-3.14E-04	6.88E-04
2P	-2.96E-07	-5.70E-06	2.28E-04	6.57E-03
3P	-3.30E-07	7.42E-06	-1.78E-05	7.57E-05
4P	-8.51E-07	2.12E-05	-1.31E-04	2.50E-04
5P	-4.46E-06	1.03E-04	-5.82E-04	8.63E-04
6P	7.32E-05	-1.85E-03	1.27E-02	-3.79E-03
7P	-4.84E-05	1.26E-03	-7.51E-03	1.47E-02
8P	-6.78E-06	-3.55E-04	9.27E-03	1.01E-02
1MA	-1.60E-07	3.77E-06	-1.60E-05	2.42E-05
2MA	-1.67E-07	4.18E-06	-1.95E-05	2.87E-05
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	2.44E-10	8.36E-09	-7.88E-08	1.33E-07
5MA	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
7MA	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
MGLY	-1.06E-05	1.74E-04	-2.42E-05	7.27E-03
GLY	1.80E-06	-7.68E-05	9.30E-04	5.12E-03
IEPOX	-1.99E-05	6.00E-04	-3.61E-03	5.38E-03

Table S4. Averaged molecular weight (MW) of lumping species.

Species Name	MW (g mol ⁻¹)	Species Name	MW (g mol ⁻¹)	Species Name	MW (g mol ⁻¹)
1VF-aromatic	216.0	1VF-terpene	216.0	1VF-isoprene	216.0
2VF-aromatic	199.0	2VF-terpene	199.0	2VF-isoprene	199.0
3VF-aromatic	182.0	3VF-terpene	182.0	3VF-isoprene	182.0
4VF-aromatic	164.0	4VF-terpene	164.0	4VF-isoprene	164.0
5VF-aromatic	147.0	5VF-terpene	147.0	5VF-isoprene	147.0
6VF-aromatic	156.0	6VF-terpene	156.0	6VF-isoprene	156.0
7VF-aromatic	149.0	7VF-terpene	149.0	7VF-isoprene	149.0
8VF-aromatic	95.0	8VF-terpene	95.0	8VF-isoprene	95.0
1F-aromatic	234.0	1F-terpene	234.0	1F-isoprene	234.0
2F-aromatic	217.0	2F-terpene	217.0	2F-isoprene	217.0
3F-aromatic	199.0	3F-terpene	199.0	3F-isoprene	199.0
4F-aromatic	192.0	4F-terpene	192.0	4F-isoprene	192.0
5F-aromatic	163.0	5F-terpene	163.0	5F-isoprene	163.0
6F-aromatic	148.0	6F-terpene	148.0	6F-isoprene	148.0
7F-aromatic	128.0	7F-terpene	128.0	7F-isoprene	128.0
8F-aromatic	110.0	8F-terpene	110.0	8F-isoprene	110.0
1M-aromatic	193.0	1M-terpene	193.0	1M-isoprene	193.0
2M-aromatic	183.0	2M-terpene	183.0	2M-isoprene	183.0
3M-aromatic	172.0	3M-terpene	172.0	3M-isoprene	172.0
4M-aromatic	196.0	4M-terpene	196.0	4M-isoprene	196.0
5M-aromatic	152.0	5M-terpene	152.0	5M-isoprene	152.0
6M-aromatic	141.0	6M-terpene	141.0	6M-isoprene	141.0
7M-aromatic	131.0	7M-terpene	131.0	7M-isoprene	131.0
8M-aromatic	121.0	8M-terpene	121.0	8M-isoprene	121.0
1S-aromatic	207.0	1S-terpene	207.0	1S-isoprene	207.0
2S-aromatic	192.0	2S-terpene	192.0	2S-isoprene	192.0
3S-aromatic	176.0	3S-terpene	176.0	3S-isoprene	176.0
4S-aromatic	160.0	4S-terpene	160.0	4S-isoprene	160.0
5S-aromatic	145.0	5S-terpene	145.0	5S-isoprene	145.0
6S-aromatic	129.0	6S-terpene	129.0	6S-isoprene	129.0
7S-aromatic	113.0	7S-terpene	113.0	7S-isoprene	113.0
8S-aromatic	98.0	8S-terpene	98.0	8S-isoprene	98.0
1P-aromatic	257.0	1P-terpene	257.0	1P-isoprene	257.0
2P-aromatic	232.0	2P-terpene	232.0	2P-isoprene	232.0
3P-aromatic	208.0	3P-terpene	208.0	3P-isoprene	208.0
4P-aromatic	183.0	4P-terpene	183.0	4P-isoprene	183.0
5P-aromatic	158.0	5P-terpene	158.0	5P-isoprene	158.0
6P-aromatic	133.0	6P-terpene	133.0	6P-isoprene	133.0
7P-aromatic	109.0	7P-terpene	109.0	7P-isoprene	109.0
8P-aromatic	84.0	8P-terpene	84.0	8P-isoprene	84.0
1MA-aromatic	257.0	1MA-terpene	257.0	1MA-isoprene	257.0
2MA-aromatic	232.0	2MA-terpene	232.0	2MA-isoprene	232.0
3MA-aromatic	208.0	3MA-terpene	208.0	3MA-isoprene	208.0
4MA-aromatic	183.0	4MA-terpene	183.0	4MA-isoprene	183.0
5MA-aromatic	158.0	5MA-terpene	158.0	5MA-isoprene	158.0
6MA-aromatic	133.0	6MA-terpene	133.0	6MA-isoprene	133.0
7MA-aromatic	109.0	7MA-terpene	109.0	7MA-isoprene	109.0
8MA-aromatic	84.0	8MA-terpene	84.0	8MA-isoprene	84.0
MGLY-aromatic	72.1	MGLY-terpene	72.1	MGLY-isoprene	72.1
GLY-aromatic	58.0	GLY-terpene	58.0	GLY-isoprene	58.0
				IEPOXY-isoprene	118.1

Table S5. Averaged Hydrogen bonding parameter (HB) of lumping species.

Species Name	HB	Species Name	HB	Species Name	HB
1VF-aromatic	1.7	1VF-terpene	3.0	1VF-isoprene	0.0
2VF-aromatic	1.5	2VF-terpene	2.6	2VF-isoprene	0.0
3VF-aromatic	1.3	3VF-terpene	1.0	3VF-isoprene	0.0
4VF-aromatic	1.1	4VF-terpene	2.0	4VF-isoprene	2.0
5VF-aromatic	0.9	5VF-terpene	0.7	5VF-isoprene	0.0
6VF-aromatic	0.1	6VF-terpene	0.0	6VF-isoprene	1.0
7VF-aromatic	0.5	7VF-terpene	0.9	7VF-isoprene	1.0
8VF-aromatic	0.3	8VF-terpene	0.0	8VF-isoprene	0.0
1F-aromatic	1.7	1F-terpene	0.0	1F-isoprene	0.0
2F-aromatic	1.5	2F-terpene	0.0	2F-isoprene	0.0
3F-aromatic	1.2	3F-terpene	0.0	3F-isoprene	0.0
4F-aromatic	0.9	4F-terpene	1.0	4F-isoprene	2.0
5F-aromatic	0.7	5F-terpene	1.0	5F-isoprene	0.0
6F-aromatic	0.4	6F-terpene	1.0	6F-isoprene	1.0
7F-aromatic	0.2	7F-terpene	0.0	7F-isoprene	1.0
8F-aromatic	0.0	8F-terpene	0.0	8F-isoprene	0.0
1M-aromatic	2.0	1M-terpene	3.0	1M-isoprene	4.0
2M-aromatic	1.7	2M-terpene	2.2	2M-isoprene	3.0
3M-aromatic	1.4	3M-terpene	1.1	3M-isoprene	3.0
4M-aromatic	0.9	4M-terpene	1.1	4M-isoprene	2.0
5M-aromatic	0.9	5M-terpene	0.2	5M-isoprene	1.8
6M-aromatic	0.6	6M-terpene	0.0	6M-isoprene	1.9
7M-aromatic	0.3	7M-terpene	0.1	7M-isoprene	1.0
8M-aromatic	0.0	8M-terpene	1.0	8M-isoprene	0.9
1S-aromatic	1.8	1S-terpene	3.7	1S-isoprene	0.0
2S-aromatic	1.5	2S-terpene	3.7	2S-isoprene	2.5
3S-aromatic	1.3	3S-terpene	1.9	3S-isoprene	3.0
4S-aromatic	1.1	4S-terpene	1.5	4S-isoprene	1.0
5S-aromatic	0.9	5S-terpene	1.0	5S-isoprene	2.0
6S-aromatic	0.7	6S-terpene	1.0	6S-isoprene	2.0
7S-aromatic	0.4	7S-terpene	1.1	7S-isoprene	0.9
8S-aromatic	0.2	8S-terpene	1.0	8S-isoprene	1.2
1P-aromatic	2.2	1P-terpene	3.6	1P-isoprene	4.0
2P-aromatic	1.9	2P-terpene	2.8	2P-isoprene	3.9
3P-aromatic	1.6	3P-terpene	3.0	3P-isoprene	2.1
4P-aromatic	1.2	4P-terpene	2.4	4P-isoprene	3.0
5P-aromatic	0.9	5P-terpene	2.0	5P-isoprene	1.5
6P-aromatic	0.5	6P-terpene	1.4	6P-isoprene	1.4
7P-aromatic	0.2	7P-terpene	0.0	7P-isoprene	2.0
8P-aromatic	0.0	8P-terpene	0.8	8P-isoprene	0.8
1MA-aromatic	2.2	1MA-terpene	0.0	1MA-isoprene	5.0
2MA-aromatic	1.9	2MA-terpene	3.0	2MA-isoprene	4.0
3MA-aromatic	1.6	3MA-terpene	0.0	3MA-isoprene	0.0
4MA-aromatic	1.2	4MA-terpene	1.0	4MA-isoprene	3.0
5MA-aromatic	0.9	5MA-terpene	0.0	5MA-isoprene	0.0
6MA-aromatic	0.5	6MA-terpene	0.0	6MA-isoprene	0.0
7MA-aromatic	0.2	7MA-terpene	0.0	7MA-isoprene	0.0
8MA-aromatic	0.0	8MA-terpene	0.0	8MA-isoprene	0.0
MGLY-aromatic	0.0	MGLY-terpene	0.0	MGLY-isoprene	0.0
GLY-aromatic	0.0	GLY-terpene	0.0	GLY-isoprene	0.0
				IEPOXY-isoprene	2.0

Table S6. Averaged Oxygen to carbon ratio (O:C) of lumping species.

Species Name	O:C	Species Name	O:C	Species Name	O:C
1VF-aromatic	0.9	1VF-terpene	0.8	1VF-isoprene	0.4
2VF-aromatic	0.9	2VF-terpene	1.2	2VF-isoprene	0.4
3VF-aromatic	0.9	3VF-terpene	1.6	3VF-isoprene	0.4
4VF-aromatic	0.8	4VF-terpene	1.3	4VF-isoprene	1.6
5VF-aromatic	0.8	5VF-terpene	0.7	5VF-isoprene	0.4
6VF-aromatic	0.4	6VF-terpene	0.7	6VF-isoprene	1.0
7VF-aromatic	0.5	7VF-terpene	0.8	7VF-isoprene	1.0
8VF-aromatic	0.7	8VF-terpene	0.8	8VF-isoprene	0.8
1F-aromatic	1.0	1F-terpene	0.4	1F-isoprene	0.4
2F-aromatic	1.0	2F-terpene	0.4	2F-isoprene	0.4
3F-aromatic	0.9	3F-terpene	0.4	3F-isoprene	0.4
4F-aromatic	0.7	4F-terpene	0.3	4F-isoprene	1.0
5F-aromatic	0.8	5F-terpene	0.5	5F-isoprene	0.4
6F-aromatic	0.4	6F-terpene	0.7	6F-isoprene	1.0
7F-aromatic	0.7	7F-terpene	0.6	7F-isoprene	0.8
8F-aromatic	0.7	8F-terpene	0.7	8F-isoprene	0.8
1M-aromatic	1.2	1M-terpene	0.6	1M-isoprene	0.9
2M-aromatic	1.1	2M-terpene	0.5	2M-isoprene	1.3
3M-aromatic	1.1	3M-terpene	0.5	3M-isoprene	1.0
4M-aromatic	1.0	4M-terpene	0.5	4M-isoprene	0.9
5M-aromatic	0.9	5M-terpene	0.6	5M-isoprene	0.7
6M-aromatic	0.8	6M-terpene	0.2	6M-isoprene	0.8
7M-aromatic	0.7	7M-terpene	0.7	7M-isoprene	0.9
8M-aromatic	0.6	8M-terpene	1.3	8M-isoprene	0.5
1S-aromatic	0.9	1S-terpene	1.1	1S-isoprene	0.4
2S-aromatic	0.9	2S-terpene	1.0	2S-isoprene	0.9
3S-aromatic	0.9	3S-terpene	0.7	3S-isoprene	1.0
4S-aromatic	0.9	4S-terpene	0.5	4S-isoprene	0.6
5S-aromatic	0.8	5S-terpene	0.6	5S-isoprene	1.4
6S-aromatic	0.8	6S-terpene	0.3	6S-isoprene	1.1
7S-aromatic	0.8	7S-terpene	0.9	7S-isoprene	1.0
8S-aromatic	0.8	8S-terpene	0.6	8S-isoprene	1.1
1P-aromatic	1.2	1P-terpene	0.8	1P-isoprene	1.0
2P-aromatic	1.1	2P-terpene	0.5	2P-isoprene	0.9
3P-aromatic	0.9	3P-terpene	0.9	3P-isoprene	1.3
4P-aromatic	0.8	4P-terpene	0.5	4P-isoprene	1.0
5P-aromatic	0.7	5P-terpene	0.3	5P-isoprene	1.4
6P-aromatic	0.5	6P-terpene	1.5	6P-isoprene	0.8
7P-aromatic	0.4	7P-terpene	0.4	7P-isoprene	0.7
8P-aromatic	0.2	8P-terpene	1.7	8P-isoprene	0.6
1MA-aromatic	1.2	1MA-terpene	0.4	1MA-isoprene	1.2
2MA-aromatic	1.1	2MA-terpene	0.6	2MA-isoprene	1.1
3MA-aromatic	0.9	3MA-terpene	0.4	3MA-isoprene	0.4
4MA-aromatic	0.8	4MA-terpene	0.7	4MA-isoprene	1.0
5MA-aromatic	0.7	5MA-terpene	0.4	5MA-isoprene	0.4
6MA-aromatic	0.5	6MA-terpene	0.4	6MA-isoprene	0.4
7MA-aromatic	0.4	7MA-terpene	0.4	7MA-isoprene	0.4
8MA-aromatic	0.2	8MA-terpene	0.4	8MA-isoprene	0.4
MGLY-aromatic	0.7	MGLY-terpene	0.7	MGLY-isoprene	0.7
GLY-aromatic	1.0	GLY-terpene	1.0	GLY-isoprene	1.0
				IEPOXY-isoprene	1.7

Table S7. Reactivity scale (*R*) of lumping species.

Species Name	<i>R</i>	Species Name	<i>R</i>	Species Name	<i>R</i>
1VF-aromatic	8.5	1VF-terpene	8.5	1VF-isoprene	8.5
2VF-aromatic	8.5	2VF-terpene	8.5	2VF-isoprene	8.5
3VF-aromatic	8.5	3VF-terpene	8.5	3VF-isoprene	8.5
4VF-aromatic	8.5	4VF-terpene	8.5	4VF-isoprene	8.5
5VF-aromatic	8.5	5VF-terpene	8.5	5VF-isoprene	8.5
6VF-aromatic	8.5	6VF-terpene	8.5	6VF-isoprene	8.5
7VF-aromatic	8.5	7VF-terpene	8.5	7VF-isoprene	8.5
8VF-aromatic	8.5	8VF-terpene	8.5	8VF-isoprene	8.5
1F-aromatic	8.2	1F-terpene	8.2	1F-isoprene	8.2
2F-aromatic	8.2	2F-terpene	8.2	2F-isoprene	8.2
3F-aromatic	8.2	3F-terpene	8.2	3F-isoprene	8.2
4F-aromatic	8.2	4F-terpene	8.2	4F-isoprene	8.2
5F-aromatic	8.2	5F-terpene	8.2	5F-isoprene	8.2
6F-aromatic	8.2	6F-terpene	8.2	6F-isoprene	8.2
7F-aromatic	8.2	7F-terpene	8.2	7F-isoprene	8.2
8F-aromatic	8.2	8F-terpene	8.2	8F-isoprene	8.2
1M-aromatic	4.0	1M-terpene	4.0	1M-isoprene	4.0
2M-aromatic	4.0	2M-terpene	4.0	2M-isoprene	4.0
3M-aromatic	4.0	3M-terpene	4.0	3M-isoprene	4.0
4M-aromatic	4.0	4M-terpene	4.0	4M-isoprene	4.0
5M-aromatic	4.0	5M-terpene	4.0	5M-isoprene	4.0
6M-aromatic	4.0	6M-terpene	4.0	6M-isoprene	4.0
7M-aromatic	4.0	7M-terpene	4.0	7M-isoprene	4.0
8M-aromatic	4.0	8M-terpene	4.0	8M-isoprene	4.0
1S-aromatic	1.0	1S-terpene	1.0	1S-isoprene	1.0
2S-aromatic	1.0	2S-terpene	1.0	2S-isoprene	1.0
3S-aromatic	1.0	3S-terpene	1.0	3S-isoprene	1.0
4S-aromatic	1.0	4S-terpene	1.0	4S-isoprene	1.0
5S-aromatic	1.0	5S-terpene	1.0	5S-isoprene	1.0
6S-aromatic	1.0	6S-terpene	1.0	6S-isoprene	1.0
7S-aromatic	1.0	7S-terpene	1.0	7S-isoprene	1.0
8S-aromatic	1.0	8S-terpene	1.0	8S-isoprene	1.0
1P-aromatic	0.0	1P-terpene	0.0	1P-isoprene	0.0
2P-aromatic	0.0	2P-terpene	0.0	2P-isoprene	0.0
3P-aromatic	0.0	3P-terpene	0.0	3P-isoprene	0.0
4P-aromatic	0.0	4P-terpene	0.0	4P-isoprene	0.0
5P-aromatic	0.0	5P-terpene	0.0	5P-isoprene	0.0
6P-aromatic	0.0	6P-terpene	0.0	6P-isoprene	0.0
7P-aromatic	0.0	7P-terpene	0.0	7P-isoprene	0.0
8P-aromatic	0.0	8P-terpene	0.0	8P-isoprene	0.0
1MA-aromatic	0.0	1MA-terpene	0.0	1MA-isoprene	0.0
2MA-aromatic	0.0	2MA-terpene	0.0	2MA-isoprene	0.0
3MA-aromatic	0.0	3MA-terpene	0.0	3MA-isoprene	0.0
4MA-aromatic	0.0	4MA-terpene	0.0	4MA-isoprene	0.0
5MA-aromatic	0.0	5MA-terpene	0.0	5MA-isoprene	0.0
6MA-aromatic	0.0	6MA-terpene	0.0	6MA-isoprene	0.0
7MA-aromatic	0.0	7MA-terpene	0.0	7MA-isoprene	0.0
8MA-aromatic	0.0	8MA-terpene	0.0	8MA-isoprene	0.0
MGLY-aromatic	9.0	MGLY-terpene	9.0	MGLY-isoprene	9.0
GLY-aromatic	12.5	GLY-terpene	12.5	GLY-isoprene	12.5
				IEPOXY-isoprene	2

Table S8. The basicity constant (pK_{BH}) of lumping species.

Species Name	pK_{BH}	Species Name	pK_{BH}	Species Name	pK_{BH}
1VF-aromatic	-1.5	1VF-terpene	-1.5	1VF-isoprene	-1.5
2VF-aromatic	-1.5	2VF-terpene	-1.5	2VF-isoprene	-1.5
3VF-aromatic	-1.5	3VF-terpene	-1.5	3VF-isoprene	-1.5
4VF-aromatic	-1.5	4VF-terpene	-1.5	4VF-isoprene	-1.5
5VF-aromatic	-1.5	5VF-terpene	-1.5	5VF-isoprene	-1.5
6VF-aromatic	-1.5	6VF-terpene	-1.5	6VF-isoprene	-1.5
7VF-aromatic	-1.5	7VF-terpene	-1.5	7VF-isoprene	-1.5
8VF-aromatic	-1.5	8VF-terpene	-1.5	8VF-isoprene	-1.5
1F-aromatic	-1.5	1F-terpene	-1.5	1F-isoprene	-1.5
2F-aromatic	-1.5	2F-terpene	-1.5	2F-isoprene	-1.5
3F-aromatic	-1.5	3F-terpene	-1.5	3F-isoprene	-1.5
4F-aromatic	-1.5	4F-terpene	-1.5	4F-isoprene	-1.5
5F-aromatic	-1.5	5F-terpene	-1.5	5F-isoprene	-1.5
6F-aromatic	-1.5	6F-terpene	-1.5	6F-isoprene	-1.5
7F-aromatic	-1.5	7F-terpene	-1.5	7F-isoprene	-1.5
8F-aromatic	-1.5	8F-terpene	-1.5	8F-isoprene	-1.5
1M-aromatic	-1.5	1M-terpene	-1.5	1M-isoprene	-1.5
2M-aromatic	-1.5	2M-terpene	-1.5	2M-isoprene	-1.5
3M-aromatic	-1.5	3M-terpene	-1.5	3M-isoprene	-1.5
4M-aromatic	-1.5	4M-terpene	-1.5	4M-isoprene	-1.5
5M-aromatic	-1.5	5M-terpene	-1.5	5M-isoprene	-1.5
6M-aromatic	-1.5	6M-terpene	-1.5	6M-isoprene	-1.5
7M-aromatic	-1.5	7M-terpene	-1.5	7M-isoprene	-1.5
8M-aromatic	-1.5	8M-terpene	-1.5	8M-isoprene	-1.5
1S-aromatic	-2.0	1S-terpene	-2.0	1S-isoprene	-2.0
2S-aromatic	-2.0	2S-terpene	-2.0	2S-isoprene	-2.0
3S-aromatic	-2.0	3S-terpene	-2.0	3S-isoprene	-2.0
4S-aromatic	-2.0	4S-terpene	-2.0	4S-isoprene	-2.0
5S-aromatic	-2.0	5S-terpene	-2.0	5S-isoprene	-2.0
6S-aromatic	-2.0	6S-terpene	-2.0	6S-isoprene	-2.0
7S-aromatic	-2.0	7S-terpene	-2.0	7S-isoprene	-2.0
8S-aromatic	-2.0	8S-terpene	-2.0	8S-isoprene	-2.0
1P-aromatic	0.0	1P-terpene	0.0	1P-isoprene	0.0
2P-aromatic	0.0	2P-terpene	0.0	2P-isoprene	0.0
3P-aromatic	0.0	3P-terpene	0.0	3P-isoprene	0.0
4P-aromatic	0.0	4P-terpene	0.0	4P-isoprene	0.0
5P-aromatic	0.0	5P-terpene	0.0	5P-isoprene	0.0
6P-aromatic	0.0	6P-terpene	0.0	6P-isoprene	0.0
7P-aromatic	0.0	7P-terpene	0.0	7P-isoprene	0.0
8P-aromatic	0.0	8P-terpene	0.0	8P-isoprene	0.0
1MA-aromatic	-2.0	1MA-terpene	-2.0	1MA-isoprene	-2.0
2MA-aromatic	-2.0	2MA-terpene	-2.0	2MA-isoprene	-2.0
3MA-aromatic	-2.0	3MA-terpene	-2.0	3MA-isoprene	-2.0
4MA-aromatic	-2.0	4MA-terpene	-2.0	4MA-isoprene	-2.0
5MA-aromatic	-2.0	5MA-terpene	-2.0	5MA-isoprene	-2.0
6MA-aromatic	-2.0	6MA-terpene	-2.0	6MA-isoprene	-2.0
7MA-aromatic	-2.0	7MA-terpene	-2.0	7MA-isoprene	-2.0
8MA-aromatic	-2.0	8MA-terpene	-2.0	8MA-isoprene	-2.0
MGLY-aromatic	-1.5	MGLY-terpene	-1.5	MGLY-isoprene	-1.5
GLY-aromatic	-1.5	GLY-terpene	-1.5	GLY-isoprene	-1.5
				IEPOXY-isoprene	-1.5

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