**Supplementary material**

# Dual roles of inorganic aqueous phase on SOA growth from benzene and phenol

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**Section S1. Time profile of sunlight intensity, temperature, relative humidity in the UF-APHOR chamber on October 19, 2022.**

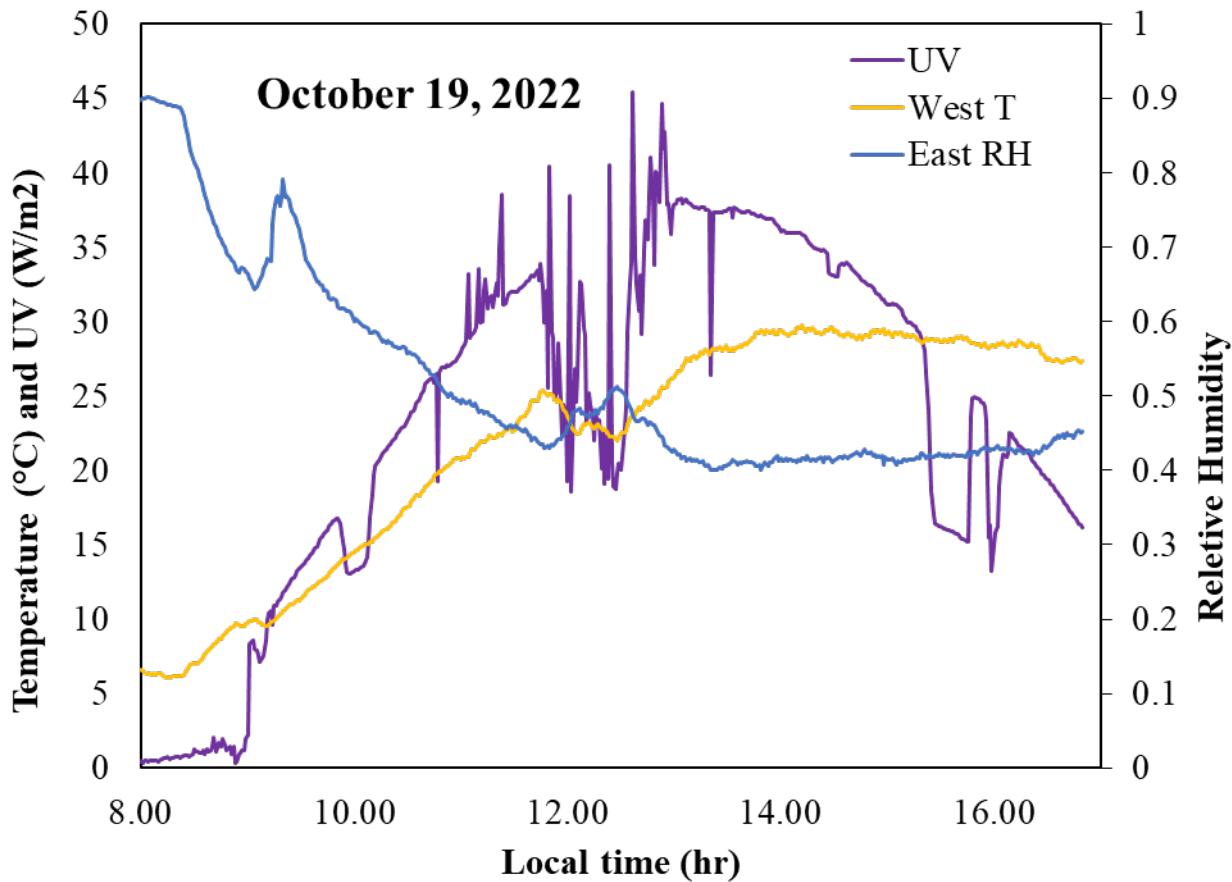



Figure S1. Time series data of sunlight intensity, temperature, and relative humidity in UF-APHOR chamber on October 19, 2022.  This sunlight profiles has been used to simulate the sensitivity of the UNIPAR model to major variables such as temperature, humidity, and $NO_x$ levels, and seed types.

**Section S2. UNIPAR Model Structure**

**S2A. UNIPAR model description**

**(1) Gas Products Lumping Structure**

The oxidation of phenol and benzene was simulated using the explicit gas mechanisms including MCM, v3.3.1 (Jenkin et al., 1997; Saunders et al., 2003; Jenkin et al., 2003), the mechanisms to form low-volatile HOM (Section 3.1.1), and the mechanisms to form PPR (Section 3.1.2) in the box model platform. The $NO_x$ dependence of gas phase products was simulated with various $HC/NO_x$ conditions (2-32 ppbC/ppb) under the same meteorological conditions (sunlight intensity, temperature, relative humidity) as on June 19, 2015. The resulting products were lumped into 50 lumping groups based on volatility and reactivity. This mass base 2D lumping array consists of 8 levels of volatility ($10^{-8}$, $10^{-6}$, $10^{-5}$, $10^{-4}$, $10^{-3}$, $10^{-2}$, $10^{-1}$, and 1 mmHg), 6 levels of aerosol phase reactivity (very fast (VF), fast (F), medium (M), slow (S), partitioning only (P), and multi-alcohol (MA)) and two additional reactive species (glyoxal (GLY), methylglyoxal (MGLY)) which are separately treated in UNIPAR model. The detailed products distribution was shown in SI tables S1-S2. The stoichiometric coefficient of resulting products are linked to the mathematical equation and applied to construct product array.

In addition, the mass based stoichiometric coefficient ($\alpha_i$) of lumping group $i$ in each $NO_x$ levels is calculated with a fractional aging scale ($f'_A(t)$) ranging from 0 to 1, which is converted by the aging factor ($f_A(t)$).

$$f_A(t) = \frac{\log[HO_2]+[RO_2]}{[HC]_0} \tag{Eq.1}$$

$$f'_A(t) = \frac{f_A(aged)-f_A(t)}{f_A(aged)-f_A(fresh)} \tag{Eq.2}$$

$$\alpha_i = \left(1 - f'_A(t)\right)(fresh\ \alpha_i) + (f'_A(t))(aged\ \alpha_i) \tag{Eq.3}$$

In the equations above, $[HO_2]$ and $[RO_2]$ are the concentration of $HO_2$ and $RO_2$ radicals (in ppb) and $[HC]$ represents the initial HC concentration (in ppbC). When the time ($t$) is small (fresh), (Eq.1) sets the lower boundary of $f_A(t)$. On the contrary, when $t$ is big (aged), the upper boundary of $f_A(t)$ was decided. The fresh $\alpha_i$ and aged $\alpha_i$ be determined, respectively. As increasing aerosol acidity, the distribution of products is less aged due to the impact of PPR on gas oxidation (retarded production of $[HO_2]$ and $[RO_2]$).

**(2) Concentrations of Species in Multiphase**

In the presence of wet-inorganic seed aerosol, the lumped products produced gas phase are separate into *g*, *or* and *in* phases by gas-aerosol absorptive partitioning model (Pankow, 1994). The *g-or* partitioning coefficient ($K_{or,i}$) (in m$^3$ µg$^{-1}$) and *g-in* partitioning coefficient ($K_{in,i}$) are expressed as (Eq.4) and (Eq.5), respectively.

$$K_{or,i} = \frac{7.501RT}{10^9 MW_{or}\gamma_{or,i}p^\circ_{l,i}} \tag{Eq.4}$$

$$K_{in,i} = \frac{7.501RT}{10^9 MW_{in}\gamma_{in,i}p^\circ_{l,i}}$$ (Eq.5)

R stands for the gas constant (8.314 J mol$^{-1}$ K$^{-1}$). MW$_{in}$ represents the average MW (g mol$^{-1}$) of inorganic aerosol. $p^\circ_{l,i}$ is the liquid vapor pressure (in mmHg) of the product $i$ and is calculated using the group contribution method (Zhao et al., 1999). The activity coefficient ($\gamma_{or,i}$) of organic species $i$ in $or$ phase is treated as one (Im et al., 2014). The activity coefficient of $i$ in $in$ ($\gamma_{in,i}$) is predicted using a semi-empirically regression equation (Zhou et al., 2019). The theoretical $\gamma_{in,i}$ was estimated by using the thermodynamic Aerosol Inorganic-Organic Mixtures Functional Groups Activity Coefficients (AIOMFAC) (Zuend et al., 2011) for given set of conditions and aerosol parameters. $\gamma_{in,i}$ is a function of aerosol environment variables (RH ranging from 0 to 1 and fractional sulfate (FS = [SO$_4^{2-}$]/[SO$_4^{2-}$]+[NH$_4^+$])) and the physicochemical parameters of species $i$ such as the molecular weight (MW$_i$), the oxygen to carbon ratio (O:C$_i$), hydrogen bonding (HB$_i$) as follows,

$$\gamma_{in,i} = e^{0.035\cdot MW_i - 2.704\cdot \ln(O:C_i) - 1.121\cdot HB_i - 0.330\cdot FS - 0.022\cdot(100\cdot RH)}$$ (Eq.6)

$K_{or,i}$ and $K_{in,i}$ were applied to estimate the concentration (μg m$^{-3}$) of the lumping species in each phase (Fig. 1).

### (3) Aerosol Phase Reaction

OM$_{AR,i}$ (in μg m$^{-3}$) forms via oligomerization in both $or$ and $in$ phases based on a second-order dimerization (Odian, 2004). The formed OM$_{AR}$ is assumed to be nonvolatile and irreversible (Kleindienst and Bullock, 2006; Cao and Jang, 2010; Zhou et al., 2019). Oligomerization in the aqueous phase can be accelerated by acid-catalyzed reactions (Jang et al., 2002) and expressed as

$$\frac{dC_{or,i}}{dt} = -k_{or,i}C'^2_{or,i}\left(\frac{MW_i OM_T}{\rho_{or}10^3}\right)$$ (Eq.7)

$$\frac{dC_{in,i}}{dt} = -k_{in,i}C'^2_{in,i}\left(\frac{MW_i M_{in}}{\rho_{in}10^3}\right)$$ (Eq.8)

k$_{or,i}$ (L mol$^{-1}$ s$^{-1}$) and k$_{in,i}$ are oligomerization rate constants in $or$ and $in$ phases, respectively. The average density of phenol and benzene aerosols ($\rho_{or}$) is 1.4 g cm$^{-3}$ (Yee et al., 2013; Nakao et al., 2013; Nakao et al., 2011; Ng et al., 2007; Borrás and Tortajada-Genaro, 2012). The density of inorganic aerosol ($\rho_{in}$ in g cm$^{-3}$) was calculated from a regression equation through the Extended Aerosol Inorganic Model (E-AIM) . The terms in brackets are conversion factors from aerosol-based concentrations ($C'_{or,i}$ and $C'_{in,I}$, mol L$^{-1}$) to air-based concentration (μg m$^{-3}$). k$_{or,i}$ (L mol$^{-1}$ s$^{-1}$) and k$_{in,i}$ are semi-empirically estimated as a function of species reactivity (R$_i$), protonation equilibrium constant (pK$_{BH^+,i}$), excess acidity (X), water activity (a$_w$), and proton concentration ([H$^+$]) using the method developed by Jang et al. shown in (Eq.9) and (Eq.10) (Jang et al., 2005; Han and Jang, 2022; Beardsley et al., 2013; Zhou et al., 2019; Yu et al., 2021).

$$k_{o,i} = 10^{0.846R_i + 0.22pK_{BH^+i} - 4.9}$$ (Eq.9)

$$k_{AC,i} = 10^{0.846R_i + 0.22pK_{BH^+i} + 1.003X + \log(a_w[H^+]) - 2.8}$$ (Eq.10)

OM$_{AR,i}$ in multiphase is calculated via a analytical solution of Eqs.11 and 12 (Im et al., 2014).

## (4) Newtonian Method to Estimate Organic Mass via Partitioning

Schell et al. developed a partitioning model to predict SOA formation which Cao and Jang reconstructed to include OM formed via aerosol-phase reactions ($OM_{AR,i}$ in µg m$^{-3}$) from total species, $i$ ($C_{T,i}$ in µg m$^{-3}$) (Schell et al., 2001; Cao and Jang, 2010). Mass balance equations as a function of the effective saturation concentration were employed to estimate the OM concentration formed from the total species during the partitioning process ($OM_P$ in µg m$^{-3}$).

$$OM_P = \sum_{ij}\left[C_{T,i} - OM_{AR,i} - C_{g,i}^o \frac{\frac{C_{or,i}}{MW_i}}{\sum_{ij}\left(\frac{C'_{or,i}}{MW_i}+\frac{OM_{AR,i}}{MW_{oli,i}}\right)+\frac{OM_0}{MW_{oli,i}}}\right] \qquad \text{(Eq.11)}$$

In (Eq.11), $MW_{oli,i}$ is the MW from oligomerization (in g mol$^{-1}$) and $OM_0$ is the concentration of the preexisting OM (in mol m$^{-3}$). $OM_p$ was solved for with the iteration method using the globally converging Newton-Raphson method (Press et al., 1996) at the end each step.

## (5) Organosulfate Formation

In the presence of acidic aerosol, UNIPAR predicts the diorganosulfate (diOS) formation to calculate the change in aerosol hygroscopicity and acidity. For example, SA can be neutralized by ammonium or converted to diOS. Sulfate is applied into a semi-empirical equation as a function of free sulfate (Im et al., 2014; Beardsley and Jang, 2016). The PIL-IC experimental data provide ammonium ion concentrations and used for the calculation of aerosol acidity and diOS formation for SOA simulation as shown in (Eq.12).

$$\frac{[diOS]_{model}}{[SO_4^{2-}]_{free}} = 1 - \frac{1}{1+f_{diOS}\frac{N_{diOS}}{[SO_4^{2-}]_{free}}} \qquad \text{(Eq.12)}$$

In (Eq.12), $f_{diOS}$ is the diOS conversion factor (Im et al., 2014) and $N_{diOS}$ denotes the numeric parameter for scaling lumping groups based on the effectiveness of diOS formation for each chemical species.

## S2B. Model Parameters

## (1) Physicochemical parameters

**Table S1.** Unified physicochemical parameters of lumping species from oxidation of phenol and benzene.

| Lumped species | phenol | | | benzene | | |
|---|---|---|---|---|---|---|
| | MW (g mol$^{-1}$) | O:C | H-bonding | MW (g mol$^{-1}$) | O:C | H-bonding |
| 1VF | 174.1082 | 1 | 2.6 | 174.1082 | 1 | 2.6 |
| 2VF | 219.1058 | 1.333333 | 1 | 219.1058 | 1.333333 | 1 |
| 3VF | 120.0609 | 1.666667 | 2.6 | 120.0609 | 1.666667 | 2.6 |
| 4VF | 118.09 | 1 | 2 | 118.09 | 1 | 2 |
| 5VF | 140.0936 | 0.666667 | 0 | 140.0936 | 0.666667 | 0 |
| 6VF | 115.8671 | 1 | 0.898263 | 115.9067 | 1 | 0.917916 |
| 7VF | 88.062 | 1 | 1 | 88.062 | 1 | 1 |
| 8VF | 86.0462 | 1 | 0 | 86.0462 | 1 | 0 |
| 1F | 0 | 0 | 0 | 0 | 0 | 0 |
| 2F | 0 | 0 | 0 | 0 | 0 | 0 |
| 3F | 0 | 0 | 0 | 0 | 0 | 0 |
| 4F | 144.0823 | 1 | 1.6 | 204.9864 | 1.166277 | 1.001431 |
| 5F | 118.5967 | 1.004738 | 1.990949 | 118.0894 | 1.000022 | 2 |
| 6F | 0 | 0 | 0 | 198.9037 | 1.260374 | 0.000245 |
| 7F | 116.07 | 1 | 0 | 116.07 | 1 | 4.97E-16 |
| 8F | 84.65 | 0.5 | 0 | 84.08599 | 0.5 | 0 |
| 1M | 159.5946 | 0.904116 | 3.747486 | 147.7398 | 1.018893 | 3.646408 |
| 2M | 142.11 | 0.666667 | 2.6 | 142.11 | 0.666667 | 2.6 |
| 3M | 125.0572 | 1.029092 | 3.037909 | 116.186 | 1.000004 | 2.607109 |
| 4M | 145.0703 | 1.25 | 1.6 | 145.0703 | 1.25 | 1.6 |
| 5M | 128.799 | 0.667997 | 1.568898 | 126.6408 | 0.525004 | 1.59185 |
| 6M | 123.3449 | 1.036167 | 0.989723 | 123.4151 | 1.037009 | 0.987718 |
| 7M | 74.03742 | 1.50006 | 1.6 | 74.03555 | 1.500002 | 1.6 |
| 8M | 71.27919 | 1.065525 | 0.564863 | 65.0994 | 1.154774 | 0.687291 |
| 1S | 0 | 0 | 0 | 0 | 0 | 0 |
| 2S | 140.094 | 0.666667 | 2 | 140.094 | 0.666667 | 2 |
| 3S | 157.4972 | 0.872951 | 1.886397 | 141.9989 | 0.996307 | 1.533303 |
| 4S | 124.1794 | 0.503462 | 1 | 124.0853 | 0.50061 | 1 |
| 5S | 161.07 | 1.5 | 0 | 161.07 | 1.5 | 0 |
| 6S | 0 | 0 | 0 | 0 | 0 | 0 |
| 7S | 108.0948 | 0.333333 | 0 | 108.0948 | 0.333333 | 0 |
| 8S | 0 | 0 | 0 | 0 | 0 | 0 |
| 1P | 155.1493 | 1.741777 | 4.562542 | 150.3565 | 2.134388 | 3.86065 |
| 2P | 185.9148 | 1.081649 | 2.743808 | 169.5117 | 0.937519 | 2.990466 |
| 3P | 184.1064 | 0.833333 | 1 | 184.1064 | 0.833333 | 1 |
| 4P | 150.8352 | 0.732435 | 2.075105 | 128.9816 | 1.201975 | 2.481655 |
| 5P | 139.1088 | 0.5 | 1 | 139.1088 | 0.5 | 1 |
| 6P | 106.7159 | 0.69126 | 1.4343 | 133.8303 | 0.792327 | 1.28921 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 7P | 110.1106 | 0.333333 | 1.6 | 142.1094 | 0.666667 | 1 |
| 8P | 84.073 | 0.5 | 0 | 92.39821 | 0.223516 | 0.829453 |
| 1MA | 169.2218 | 0.979188 | 5.098942 | 159.5576 | 0.848421 | 5.089731 |
| 2MA | 142.11 | 0.666667 | 4 | 142.11 | 0.666667 | 4 |
| 3MA | 0 | 0 | 0 | 0 | 0 | 0 |
| 4MA | 0 | 0 | 0 | 92.11 | 0.5 | 3 |
| 5MA | 0 | 0 | 0 | 0 | 0 | 0 |
| 6MA | 0 | 0 | 0 | 0 | 0 | 0 |
| 7MA | 0 | 0 | 0 | 0 | 0 | 0 |
| 8MA | 0 | 0 | 0 | 0 | 0 | 0 |
| MGLY | 0 | 0 | 0 | 0 | 0 | 0 |
| GLY | 58.0361 | 1 | 0 | 58.0361 | 1 | 0 |

## (2) Stoichiometric coefficients

The coefficients in the Tables (S2-S7) are integrated into the following mathematical equations to construct stoichiometric coefficient array of lumping species.

$$A_1 * R\_V1N^3 + A_1\_LNOX\_fresh(i) * R\_V1N^2 \ \& + A_1\_fresh(i) * R\_V1N + A_1 \qquad \text{(Eq. 13)}$$

where $R\_V1N$ is the HC ppbC/$NO_x$ ppb ratio

**Table S2.** Stoichiometric coefficient array of lumping species generated from the oxidation of phenol under the sunlight without SA for the UNIPAR model.

| | Oxidation path: phenol + OH without SA | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Lumped species | Low $NO_x$ (R_V1N $\geq$ 5) | | | | High $NO_x$ (R_V1N < 5) | | | |
| | $A_1$ | $B_1$ | $C_1$ | $D_1$ | $A_1$ | $B_1$ | $C_1$ | $D_1$ |
| 1VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2VF | 2.0766E-07 | -1.3097E-05 | 2.1637E-04 | 1.3470E-03 | -2.7092E-08 | -1.7729E-05 | 4.5989E-04 | -4.3263E-04 |
| 3VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6VF | 7.9035E-08 | -4.6010E-06 | 5.9991E-05 | 6.4261E-04 | 1.0674E-07 | -5.8088E-06 | 7.9644E-05 | 5.2590E-04 |
| 7VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5F | 3.2943E-07 | -2.9298E-05 | 8.3827E-04 | 4.1888E-03 | -3.6654E-06 | 1.5929E-04 | -2.0059E-03 | 1.7901E-02 |
| 6F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7F | 6.9208E-07 | -3.7231E-05 | 3.6665E-04 | 6.2233E-03 | 4.5054E-06 | -1.8427E-04 | 2.1984E-03 | -1.0565E-03 |
| 8F | 3.2481E-06 | -2.2302E-04 | 4.5117E-03 | 4.4345E-03 | 1.8330E-05 | -5.3990E-04 | 4.9067E-03 | 1.8265E-02 |
| 1M | -6.7149E-07 | -1.1510E-05 | 2.3269E-03 | 7.5070E-02 | 1.0425E-04 | -2.9654E-03 | 2.4701E-02 | 4.5574E-02 |
| 2M | -5.2114E-06 | 2.7051E-04 | -1.9813E-03 | 6.0931E-02 | 7.9064E-05 | -1.8536E-03 | 1.0206E-02 | 6.7842E-02 |
| 3M | 1.4711E-07 | -1.9121E-05 | 6.8469E-04 | 1.6073E-02 | 4.6980E-06 | -1.2579E-04 | 1.0701E-03 | 1.8632E-02 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 4M | 5.7778E-07 | -1.0384E-05 | -9.5318E-04 | 2.5974E-02 | -2.2103E-06 | -1.4838E-04 | 3.9223E-03 | -5.9922E-03 |
| 5M | -2.7520E-06 | 1.6694E-04 | -2.4506E-03 | 2.7819E-02 | 6.4887E-06 | -9.1579E-05 | -2.6698E-04 | 2.1763E-02 |
| 6M | -2.3238E-06 | 7.4349E-05 | 1.5573E-03 | 1.3654E-01 | -5.0510E-06 | -3.2821E-04 | 1.3656E-02 | 5.5938E-02 |
| 7M | 2.0321E-06 | -1.2938E-04 | 2.2491E-03 | 1.1644E-02 | 1.0723E-06 | -1.3205E-04 | 2.8774E-03 | 6.3892E-03 |
| 8M | -2.2289E-07 | 1.3125E-05 | -1.9692E-04 | 2.1221E-03 | 7.3661E-07 | -2.6192E-05 | 3.2878E-04 | -2.1454E-04 |
| 1S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2S | 8.0515E-08 | -5.1791E-06 | 8.8631E-05 | 2.3209E-03 | 8.9440E-07 | -2.1284E-05 | 7.7544E-05 | 3.3077E-03 |
| 3S | -6.1820E-08 | 3.5322E-06 | -4.5906E-05 | 2.2749E-04 | -4.1715E-08 | 2.0124E-06 | -1.4974E-05 | 3.0443E-05 |
| 4S | 1.4362E-07 | -9.4814E-06 | 1.7118E-04 | 5.8243E-03 | 2.0350E-06 | -4.6534E-05 | 1.3903E-04 | 8.1248E-03 |
| 5S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7S | 3.0179E-07 | -2.3242E-05 | 5.5786E-04 | 3.2594E-02 | -2.1753E-06 | 8.5178E-05 | -9.7760E-04 | 3.9622E-02 |
| 8S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1P | -6.4645E-07 | 1.8106E-05 | 5.2763E-04 | -4.5717E-03 | -3.2836E-06 | 1.2555E-04 | -9.1700E-04 | 1.5044E-03 |
| 2P | -3.4764E-06 | 2.2287E-04 | -3.7977E-03 | 2.1333E-02 | -4.9438E-07 | 3.7573E-05 | -3.0767E-04 | 6.0435E-04 |
| 3P | 4.5544E-08 | -2.0191E-06 | -3.8996E-06 | 1.1829E-03 | -5.4651E-08 | -5.8139E-06 | 1.4551E-04 | 1.5017E-04 |
| 4P | 2.0902E-05 | -1.1662E-03 | 1.2873E-02 | 2.5087E-01 | 2.9294E-05 | -3.5584E-03 | 6.8138E-02 | -6.1945E-02 |
| 5P | 1.5743E-06 | -7.3109E-05 | 4.8235E-05 | 5.6623E-02 | -6.9809E-06 | -2.2322E-04 | 7.9286E-03 | 2.5637E-03 |
| 6P | -2.1914E-05 | 1.3168E-03 | -1.8586E-02 | 2.3671E-01 | -1.0403E-04 | 4.2824E-03 | -5.0154E-02 | 3.2231E-01 |
| 7P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8P | -4.6166E-07 | 2.7186E-05 | -3.9515E-04 | 2.0953E-02 | 1.8031E-05 | -5.6681E-04 | 5.3563E-03 | 5.2854E-03 |
| 1MA | -6.4868E-06 | 4.0243E-04 | -6.4528E-03 | 6.1163E-02 | 7.1431E-06 | -1.1327E-04 | 1.4221E-04 | 3.1532E-02 |
| 2MA | -2.1163E-06 | 1.1144E-04 | -9.0582E-04 | 1.9559E-02 | -1.4892E-05 | 6.1160E-04 | -7.0862E-03 | 4.3110E-02 |
| 3MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| MGLY | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| GLY | 1.1516E-05 | -7.5023E-04 | 1.3399E-02 | 8.5479E-02 | 5.1907E-05 | -2.0514E-03 | 2.5959E-02 | 5.2439E-02 |

**Table S3.** Stoichiometric coefficient array of oxygenated products from the oxidation of phenol under the sunlight with SA for the UNIPAR model.

| | Oxidation path: phenol + OH with SA | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Lumped species | Low NO$_x$ | | | | High NO$_x$ | | | |
| | $A_1$ | $B_1$ | $C_1$ | $D_1$ | $A_1$ | $B_1$ | $C_1$ | $D_1$ |
| 1VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2VF | -3.4594E-08 | 2.6512E-06 | -6.4020E-05 | 6.5047E-04 | -7.3419E-07 | 1.5381E-05 | -6.7714E-05 | 1.0401E-04 |
| 3VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8F | -2.2516E-07 | 1.7834E-05 | -4.5778E-04 | 5.7682E-03 | -3.4846E-06 | 5.5382E-05 | 7.0124E-05 | -1.2963E-04 |
| 1M | -2.7275E-08 | 1.9277E-06 | -3.8238E-05 | 4.3398E-04 | -4.9267E-07 | 9.6955E-06 | -2.9508E-05 | 4.4596E-05 |
| 2M | -3.3041E-08 | 2.2244E-06 | -3.4950E-05 | 4.9960E-04 | -5.7853E-07 | 1.1127E-05 | -2.0524E-05 | 2.3881E-05 |
| 3M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4M | -1.6596E-06 | 1.3048E-04 | -3.2511E-03 | 3.4909E-02 | -1.1615E-05 | 9.8518E-05 | 1.4417E-03 | 1.3576E-03 |
| 5M | -2.5888E-06 | 1.7007E-04 | -2.0434E-03 | 7.1508E-02 | -2.0588E-05 | -2.7932E-05 | 9.9658E-03 | -1.0573E-02 |
| 6M | 2.1932E-06 | -1.9177E-04 | 5.4713E-03 | 1.0110E-01 | -5.1505E-06 | 1.8081E-04 | 3.4396E-04 | 1.2155E-01 |
| 7M | -9.1750E-08 | 6.9709E-06 | -1.6718E-04 | 4.2991E-03 | -1.4529E-06 | 2.3131E-05 | 2.8672E-05 | 2.0524E-03 |
| 8M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7S | 7.6882E-08 | -7.5916E-06 | 2.1924E-04 | 7.2760E-02 | 1.9889E-05 | -6.2890E-04 | 6.4125E-03 | 5.3094E-02 |
| 8S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2P | -8.8834E-09 | 5.9116E-07 | -6.2845E-06 | 1.7227E-04 | -1.1236E-07 | 1.5326E-06 | 1.3413E-05 | -1.1921E-05 |
| 3P | -1.9651E-07 | 1.6005E-05 | -4.1933E-04 | 4.7707E-03 | 2.9630E-07 | -2.9381E-05 | 4.0412E-04 | 6.0635E-04 |
| 4P | -3.0474E-09 | -1.1645E-05 | 4.0863E-04 | 7.2726E-01 | 1.9990E-04 | -6.3673E-03 | 6.4773E-02 | 5.1913E-01 |
| 5P | 2.8654E-06 | -1.9611E-04 | 4.0691E-03 | 2.8444E-01 | -2.7302E-04 | 9.2718E-03 | -1.0048E-01 | 6.5872E-01 |
| 6P | -1.9629E-06 | 1.5638E-04 | -3.9168E-03 | 4.8265E-02 | -1.0652E-05 | 1.9085E-06 | 3.1936E-03 | 1.3545E-03 |
| 7P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8P | -7.9313E-07 | 5.9987E-05 | -1.3717E-03 | 1.3907E-02 | -1.1363E-05 | 2.0356E-04 | -3.9335E-04 | 5.0072E-04 |
| 1MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2MA | -6.3920E-10 | -5.9913E-08 | 5.7115E-06 | 9.0706E-05 | 5.3856E-08 | -2.2021E-06 | 3.0962E-05 | 2.7302E-06 |
| 3MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| MGLY | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| GLY | 2.9570E-06 | -2.3189E-04 | 5.4447E-03 | 9.8720E-03 | -1.3145E-05 | 5.4935E-04 | -4.9025E-03 | 4.9154E-02 |

**Table S4.** Stoichiometric coefficient array of fresh, oxygenated products from the oxidation of benzene under the sunlight without SA for the UNIPAR model.

| Oxidation path: benzene + OH without SA | | | | | | | |
|---|---|---|---|---|---|---|---|
| Lumped species | Low NO$_x$ | | | | High NO$_x$ | | | |
| | A$_1$ | B$_1$ | C$_1$ | D$_1$ | A$_1$ | B$_1$ | C$_1$ | D$_1$ |
| 1VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2VF | -2.8096E-09 | 6.6597E-07 | -1.5082E-05 | 9.5787E-05 | 4.7594E-09 | -1.7838E-08 | -4.3120E-08 | 1.9081E-07 |
| 3VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6VF | -1.2139E-08 | 5.4537E-07 | -1.9853E-06 | 1.0665E-05 | -1.9499E-08 | 7.1166E-07 | -2.3902E-06 | 3.6705E-06 |
| 7VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5F | -1.6013E-07 | 8.7023E-06 | -7.2527E-05 | 5.3907E-04 | -2.8216E-07 | 9.6309E-06 | -2.5341E-05 | 4.0104E-05 |
| 6F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7F | -1.3113E-06 | 4.2492E-05 | 1.1592E-03 | 1.3422E-02 | -4.3202E-06 | 6.4009E-05 | 2.3475E-03 | 1.0696E-03 |
| 8F | 1.1554E-06 | -2.9470E-05 | -1.2617E-03 | 1.3025E-01 | 4.1068E-06 | -7.6406E-05 | -1.6878E-03 | 1.3717E-01 |
| 1M | -8.4936E-07 | 7.7954E-05 | -1.5696E-03 | 9.6022E-03 | 1.6862E-07 | 2.1075E-06 | -1.1523E-05 | 2.0462E-05 |
| 2M | -2.1143E-06 | 1.6675E-04 | -3.2573E-03 | 1.9299E-02 | 5.3170E-07 | -3.1896E-06 | 1.5719E-06 | 1.0219E-05 |
| 3M | -1.9577E-07 | 1.1194E-05 | -9.7347E-05 | 7.3196E-04 | -3.8472E-07 | 1.3161E-05 | -3.8670E-05 | 5.7347E-05 |
| 4M | 2.2279E-08 | -9.7797E-07 | 1.7037E-05 | -9.2185E-05 | -8.3304E-10 | 1.3879E-07 | -8.2404E-07 | 1.2760E-06 |
| 5M | -2.0702E-06 | 1.3922E-04 | -2.4872E-03 | 1.4161E-02 | 1.7159E-07 | 5.8843E-06 | -4.0697E-05 | 6.8317E-05 |
| 6M | -3.6132E-07 | 1.3815E-04 | -2.4108E-03 | 2.0995E-02 | -1.1162E-06 | 5.9252E-05 | 3.1704E-04 | 7.2838E-04 |
| 7M | -2.8228E-07 | 1.8048E-05 | -2.3053E-04 | 1.3777E-03 | -2.6858E-07 | 1.1115E-05 | -4.1080E-05 | 6.2786E-05 |
| 8M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2S | -2.5806E-08 | 1.5115E-06 | -1.7692E-05 | 1.0052E-04 | -2.7581E-08 | 1.0925E-06 | -4.6827E-06 | 6.4690E-06 |
| 3S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4S | -6.2736E-08 | 3.6301E-06 | -3.9872E-05 | 2.5372E-04 | -7.7030E-08 | 2.8269E-06 | -8.4150E-06 | 1.3217E-05 |
| 5S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7S | -2.7735E-07 | 1.3047E-05 | 1.1917E-05 | 1.9504E-03 | -5.8745E-07 | 1.2560E-05 | 2.1127E-04 | 1.3704E-04 |
| 8S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3P | -7.1788E-09 | 4.7806E-07 | -5.4632E-06 | 3.3436E-05 | -8.5592E-09 | 3.5877E-07 | -1.2492E-06 | 1.9546E-06 |
| 4P | 1.4971E-06 | -6.4197E-05 | 1.2686E-03 | -6.2614E-03 | -8.5536E-07 | 3.4432E-05 | -1.1469E-04 | 1.7754E-04 |
| 5P | -1.1611E-09 | -7.5198E-07 | 4.6876E-04 | 1.5472E-03 | -1.1952E-06 | 2.6275E-05 | 4.1765E-04 | 2.8203E-04 |
| 6P | -2.2796E-06 | 1.7180E-05 | 3.0425E-03 | 8.7528E-02 | -6.2805E-06 | 4.0057E-05 | 4.7605E-03 | 7.0277E-02 |
| 7P | 2.4253E-07 | -2.3513E-05 | 8.5025E-04 | 2.2063E-03 | -6.7094E-07 | -8.0488E-06 | 9.5508E-04 | 2.6400E-04 |
| 8P | 7.9088E-06 | -3.7110E-04 | -1.1205E-03 | 8.2553E-01 | 1.8685E-05 | -4.0207E-04 | -6.6894E-03 | 8.7905E-01 |
| 1MA | -1.5845E-07 | 1.0536E-05 | -1.4557E-04 | 7.3669E-04 | -4.3833E-08 | 3.8043E-06 | -2.3598E-05 | 3.6245E-05 |
| 2MA | -4.8471E-07 | 2.5091E-05 | -1.6646E-04 | 1.1966E-03 | -1.0761E-06 | 3.6733E-05 | -1.3929E-04 | 1.8282E-04 |
| 3MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4MA | -5.4104E-08 | 1.2230E-06 | 6.4131E-05 | 3.6928E-04 | -3.2711E-07 | 6.5832E-06 | 7.4429E-05 | -5.8772E-05 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 5MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| MGLY | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| GLY | -1.1020E-06 | 5.6963E-05 | -2.8675E-04 | 2.1932E-01 | -1.9315E-06 | 4.4927E-05 | 5.5594E-04 | 2.1228E-01 |

**Table S5.** Stoichiometric coefficient array of aged, oxygenated products from the oxidation of benzene under the sunlight without SA for the UNIPAR model.

| | Oxidation path: benzene + OH without SA | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Lumped species | Low NO$_x$ | | | | High NO$_x$ | | | |
| | A$_1$ | B$_1$ | C$_1$ | D$_1$ | A$_1$ | B$_1$ | C$_1$ | D$_1$ |
| 1VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2VF | -8.2681E-08 | 6.6507E-06 | -1.7858E-04 | 2.6107E-03 | -6.2419E-07 | 4.3219E-06 | 1.7603E-04 | -3.0008E-04 |
| 3VF | 4.4691E-09 | -6.1259E-07 | 2.4201E-05 | -1.9251E-04 | 3.0753E-08 | -3.0515E-07 | 5.4434E-07 | 3.2952E-07 |
| 4VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6VF | -2.2453E-07 | 1.6948E-05 | -4.2435E-04 | 3.8445E-03 | -4.6322E-07 | 7.8899E-06 | -1.3024E-05 | 5.5402E-04 |
| 7VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5F | -3.9335E-08 | 3.4059E-06 | -9.1369E-05 | 1.4440E-03 | 6.3257E-08 | 2.5292E-05 | -7.2212E-04 | 5.5743E-03 |
| 6F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7F | -3.5953E-06 | 2.6582E-04 | -6.4664E-03 | 5.4697E-02 | -1.1635E-06 | -1.5919E-05 | -2.3152E-04 | 1.6631E-02 |
| 8F | -2.1166E-06 | 1.5599E-04 | -3.7667E-03 | 3.2324E-02 | 1.4166E-05 | -3.9980E-04 | 2.3995E-03 | 9.5229E-03 |
| 1M | -5.0775E-07 | 2.5884E-05 | 1.3326E-04 | 4.0026E-03 | 1.0089E-04 | -2.8411E-03 | 2.1735E-02 | -2.0619E-02 |
| 2M | -5.2920E-07 | 3.4065E-05 | -5.7965E-04 | 6.0043E-03 | 5.7832E-05 | -1.5832E-03 | 1.1353E-02 | -8.1318E-03 |
| 3M | -3.4356E-07 | 2.1060E-05 | -2.3424E-04 | 5.2158E-03 | 2.2029E-05 | -6.4502E-04 | 5.2118E-03 | -2.8069E-03 |
| 4M | 2.1999E-06 | -5.9710E-05 | -3.0652E-03 | 1.4111E-01 | -1.9072E-04 | 4.8442E-03 | -2.5911E-02 | 3.9562E-02 |
| 5M | -1.7929E-07 | 1.4575E-05 | -3.4260E-04 | 7.9012E-03 | 8.6639E-06 | -2.8194E-04 | 2.7930E-03 | -2.4513E-03 |
| 6M | -1.4396E-06 | 1.1152E-04 | -2.5606E-03 | 6.1435E-02 | 2.3732E-05 | -9.6441E-04 | 1.1874E-02 | 2.0267E-03 |
| 7M | -4.0252E-06 | 2.9585E-04 | -7.1648E-03 | 5.9180E-02 | -1.4482E-05 | 2.9679E-04 | -1.2173E-03 | 5.9069E-03 |
| 8M | 6.4447E-07 | -5.2669E-05 | 1.5286E-03 | -7.9964E-03 | 3.1840E-06 | -8.7697E-05 | 1.0432E-03 | -1.5693E-03 |
| 1S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2S | -1.1686E-08 | 8.9287E-07 | -1.9654E-05 | 1.4033E-03 | 2.2549E-06 | -6.1829E-05 | 4.2365E-04 | 1.1374E-03 |
| 3S | 4.0136E-07 | -3.4460E-05 | 9.9247E-04 | -7.0812E-03 | 8.1178E-07 | -6.7712E-06 | 3.3655E-06 | 3.1874E-05 |
| 4S | 5.7598E-08 | -5.3180E-06 | 1.7817E-04 | 1.7947E-03 | 5.6441E-06 | -1.5090E-04 | 1.0272E-03 | 2.7462E-03 |
| 5S | -3.2807E-08 | 3.1826E-06 | -1.1329E-04 | 2.0461E-03 | -2.2709E-06 | 5.4865E-05 | -2.6336E-04 | 3.2554E-04 |
| 6S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7S | -4.9990E-07 | 3.4844E-05 | -7.3255E-04 | 1.9065E-02 | 8.0962E-06 | -2.2853E-04 | 1.5191E-03 | 1.5281E-02 |
| 8S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1P | 1.0162E-05 | -7.8149E-04 | 2.0027E-02 | -1.3253E-01 | 6.3750E-06 | 9.5480E-05 | -1.4008E-03 | 2.9418E-03 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 2P | 1.6488E-06 | -1.3359E-04 | 3.6497E-03 | -2.4840E-02 | 1.5276E-06 | 1.3982E-05 | -2.4949E-04 | 5.4524E-04 |
| 3P | 2.7406E-07 | -2.3346E-06 | -6.7471E-04 | 2.0778E-02 | -1.6767E-05 | 4.1388E-04 | -1.9715E-03 | 4.8614E-03 |
| 4P | -1.2442E-05 | 9.4897E-04 | -2.4707E-02 | 3.5372E-01 | -1.5964E-04 | 2.7386E-03 | 5.4771E-03 | 5.1843E-03 |
| 5P | -3.6689E-06 | 3.3364E-04 | -1.1065E-02 | 2.0295E-01 | -1.3200E-04 | 3.0603E-03 | -1.2826E-02 | 5.5431E-02 |
| 6P | 1.0112E-05 | -8.5927E-04 | 2.5195E-02 | -4.9321E-02 | 9.6870E-05 | -2.0938E-03 | 1.0440E-02 | 1.5124E-01 |
| 7P | 5.7397E-06 | -4.7054E-04 | 1.3355E-02 | -9.2718E-02 | 8.7848E-06 | -7.5843E-06 | -1.0509E-03 | 7.6372E-03 |
| 8P | -9.1182E-06 | 6.2982E-04 | -1.2933E-02 | 1.7278E-01 | -5.5269E-05 | 2.5501E-03 | -4.2546E-02 | 3.4038E-01 |
| 1MA | -8.3685E-08 | -1.9244E-05 | 2.0738E-03 | -8.8182E-03 | 2.3911E-05 | -5.6619E-04 | 3.5178E-03 | 1.0425E-02 |
| 2MA | -1.7522E-07 | 1.1237E-05 | -1.9015E-04 | 1.9361E-03 | -3.3980E-07 | 7.2889E-05 | -1.7225E-03 | 1.1467E-02 |
| 3MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4MA | -3.6381E-08 | 2.3528E-06 | -4.1904E-05 | 3.8505E-04 | -2.5151E-07 | 1.9157E-05 | -3.6699E-04 | 2.1866E-03 |
| 5MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| MGLY | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| GLY | -8.2527E-06 | 7.0429E-04 | -2.0076E-02 | 2.5097E-01 | 3.6943E-05 | -1.2900E-03 | 1.0129E-02 | 9.4244E-02 |

**Table S6.** Stoichiometric coefficient array of fresh, oxygenated products from the oxidation of benzene under the sunlight with SA for the UNIPAR model.

| | Oxidation path: benzene + OH with SA | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Lumped species | Low NO$_x$ | | | | High NO$_x$ | | | |
| | A$_1$ | B$_1$ | C$_1$ | D$_1$ | A$_1$ | B$_1$ | C$_1$ | D$_1$ |
| 1VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2VF | 1.1816E-09 | -2.6779E-07 | 1.9346E-05 | -1.7937E-04 | -9.8873E-09 | 6.2405E-07 | -3.4202E-06 | 5.4908E-06 |
| 3VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6VF | 1.3952E-09 | -2.7796E-07 | 1.5749E-05 | 1.5378E-04 | -2.2177E-08 | 3.8472E-07 | 2.1917E-05 | -3.5720E-05 |
| 7VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7F | 2.8491E-08 | -5.4607E-06 | 2.9059E-04 | 5.4734E-02 | 7.6815E-06 | -4.4097E-04 | 8.4424E-03 | 3.8436E-03 |
| 8F | -7.2634E-08 | 1.5142E-05 | -9.3898E-04 | 6.9353E-02 | -3.6685E-06 | 2.4011E-04 | -5.6937E-03 | 1.0336E-01 |
| 1M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4M | 4.8949E-08 | -1.0259E-05 | 6.4294E-04 | 6.9815E-04 | -6.6826E-07 | 1.9113E-05 | 4.2214E-04 | -6.9633E-04 |
| 5M | 3.4856E-08 | -7.3058E-06 | 4.7665E-04 | -2.2592E-03 | -5.3763E-07 | 2.3721E-05 | -2.4305E-05 | -1.8356E-05 |
| 6M | 1.2720E-07 | -2.9827E-05 | 2.3257E-03 | -3.6166E-03 | 4.4524E-07 | -3.0596E-05 | 1.9433E-03 | 1.5474E-03 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 7M | 1.7643E-08 | -3.6720E-06 | 2.2773E-04 | 6.9377E-04 | -2.3420E-07 | 5.5725E-06 | 1.9782E-04 | -3.0684E-04 |
| 8M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7S | 1.5658E-08 | -3.2277E-06 | 1.9714E-04 | 6.4149E-03 | 6.7168E-07 | -4.4251E-05 | 1.0672E-03 | 1.4778E-04 |
| 8S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3P | 1.0536E-08 | -2.1850E-06 | 1.3416E-04 | 3.0840E-04 | -1.2166E-07 | 2.9220E-06 | 1.0874E-04 | -1.2885E-04 |
| 4P | 4.5796E-07 | -9.4357E-05 | 5.7573E-03 | 1.7944E-01 | 1.8463E-05 | -1.2271E-03 | 2.9957E-02 | 3.8028E-03 |
| 5P | 2.3355E-07 | -4.8406E-05 | 2.9691E-03 | 1.1556E-01 | 8.7698E-06 | -5.8591E-04 | 1.4471E-02 | 3.1913E-02 |
| 6P | -5.2807E-11 | 1.5550E-06 | -3.1334E-04 | 8.5335E-02 | -1.1475E-06 | 4.0749E-05 | -3.6878E-04 | 8.0398E-02 |
| 7P | -1.0911E-08 | 2.2615E-06 | -1.3752E-04 | 1.4509E-02 | 2.8183E-06 | -1.4266E-04 | 2.1638E-03 | 3.2806E-03 |
| 8P | -7.1069E-07 | 1.4658E-04 | -8.9451E-03 | 6.1229E-01 | -2.6543E-05 | 1.7829E-03 | -4.4202E-02 | 8.7044E-01 |
| 1MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| MGLY | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| GLY | 1.0489E-08 | -2.2826E-06 | 1.5811E-04 | 2.2089E-01 | 1.9514E-06 | -1.1357E-04 | 2.2518E-03 | 2.0782E-01 |

**Table S7.** Stoichiometric coefficient array of aged, oxygenated products from the oxidation of benzene under the sunlight with SA for UNIPAR model.

| | Oxidation path: benzene + OH with SA | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Lumped species | Low NO$_x$ | | | | High NO$_x$ | | | |
| | A$_1$ | B$_1$ | C$_1$ | D$_1$ | A$_1$ | B$_1$ | C$_1$ | D$_1$ |
| 1VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2VF | 8.2907E-11 | 1.9299E-09 | -3.1343E-06 | 6.5202E-04 | 6.1044E-08 | -4.4570E-06 | 1.0224E-04 | -1.4608E-04 |
| 3VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6VF | -6.5453E-10 | 1.4359E-07 | -1.0404E-05 | 4.0958E-04 | 1.1750E-07 | -4.8013E-06 | 4.0715E-05 | 3.7377E-04 |
| 7VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8VF | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 4F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7F | -1.0974E-08 | 2.3910E-06 | -1.7017E-04 | 1.0812E-02 | -1.6978E-06 | 9.4237E-05 | -1.7903E-03 | 2.0215E-02 |
| 8F | -5.9004E-09 | 1.2770E-06 | -8.9543E-05 | 5.3936E-03 | -3.7528E-07 | 2.4790E-05 | -5.9008E-04 | 8.9520E-03 |
| 1M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4M | 1.2452E-07 | -2.3067E-05 | 9.9847E-04 | 9.7610E-02 | 1.4018E-05 | -7.4110E-04 | 1.3136E-02 | 2.7219E-02 |
| 5M | 9.7667E-11 | -5.3174E-08 | 1.0555E-05 | 4.3323E-03 | 1.0951E-06 | -5.7424E-05 | 9.5387E-04 | -5.1360E-04 |
| 6M | 3.4323E-08 | -7.3472E-06 | 5.0156E-04 | 2.1507E-02 | -5.2049E-07 | -1.5204E-05 | 1.5909E-03 | 8.0462E-03 |
| 7M | 6.7384E-10 | 7.1083E-08 | -3.6990E-05 | 6.7307E-03 | 6.6587E-07 | -3.2675E-05 | 4.8808E-04 | 3.7472E-03 |
| 8M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5S | 3.3413E-09 | -7.1046E-07 | 4.7057E-05 | -1.4064E-04 | -1.1240E-07 | 4.8267E-06 | -2.5249E-05 | 3.5646E-05 |
| 6S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7S | -5.4305E-10 | 1.1587E-07 | -8.4854E-06 | 1.3458E-02 | 5.9006E-07 | -3.0343E-05 | 4.8304E-04 | 1.0974E-02 |
| 8S | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3P | -1.6183E-08 | 4.0034E-06 | -3.6179E-04 | 2.7778E-02 | 5.5086E-06 | -2.4852E-04 | 2.9230E-03 | 1.7147E-02 |
| 4P | -2.2330E-07 | 4.6115E-05 | -2.9003E-03 | 4.0179E-01 | 3.2744E-05 | -1.5518E-03 | 1.9812E-02 | 3.1579E-01 |
| 5P | 3.3461E-08 | -6.0784E-06 | 1.8361E-04 | 2.9654E-01 | -3.2890E-05 | 1.6771E-03 | -2.6570E-02 | 4.2813E-01 |
| 6P | -2.1939E-08 | 5.2238E-06 | -4.2887E-04 | 1.1456E-01 | 7.8744E-06 | -3.7418E-04 | 4.9973E-03 | 9.2595E-02 |
| 7P | 2.8532E-09 | -7.3132E-07 | 7.1020E-05 | 2.8915E-03 | -1.2644E-06 | 5.9949E-05 | -7.9522E-04 | 6.4258E-03 |
| 8P | 5.2831E-08 | -1.5608E-05 | 1.8314E-03 | 1.1461E-01 | -3.2091E-05 | 1.5034E-03 | -1.9406E-02 | 1.9821E-01 |
| 1MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 7MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 8MA | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| MGLY | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| GLY | -3.4545E-08 | 7.5117E-06 | -5.3108E-04 | 6.9518E-02 | -4.9695E-06 | 2.8060E-04 | -5.4594E-03 | 9.8983E-02 |

## (3) Major oxygenated products in lumping groups

Reactivity scales of the oxidation products are determined according to the number of reactive functional groups in their chemical structure. The reactivity bins used in UNIPAR are very fast (VF, α-hydroxybicarbonyls and tricarbonyls), fast (F, 2 epoxides or aldehydes,), medium (M, 1 epoxide or aldehyde), slow (S, ketones), partitioning only (P) and multi-alcohol (MA, 3 or more alcohols). The explicit chemical structures of oxidation products from phenol and benzene are summarized in Table S9-S10 as examples.

**Table S8**. Major oxygenated products distribution in gas phase for phenol oxidation under aged and low NO$_x$ (HC/NO$_x$=16) condition.

| $\alpha_{m,n}$ | | Phenol: Vapor Pressure (mmHg) [n] | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | n = 1 ($10^{-8}$) | n = 2 ($10^{-6}$) | n = 3 ($10^{-5}$) | n = 4 ($10^{-4}$) | n = 5 ($10^{-3}$) | n = 6 ($10^{-2}$) | n = 7 ($10^{-1}$) | n = 8 ($10^0$) |
| Reactivity [m] | VF | | | | | | | | |
| | F | | | | | | | | |
| | M | | | | | | | | |
| | S | | | | | | | | |
| | P | | | | | | | | |
| | MA | | | | | | | | |
| | R | | | | | | | | GLY |

**Table S9**. Major oxygenated products distribution in gas phase for benzene oxidation under aged and low NO$_x$ (HC/NO$_x$=14) condition.

| $\alpha_{m,n}$ | | Benzene: Vapor Pressure (mmHg) [n] | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | n = 1 ($10^{-8}$) | n = 2 ($10^{-6}$) | n = 3 ($10^{-5}$) | n = 4 ($10^{-4}$) | n = 5 ($10^{-3}$) | n = 6 ($10^{-2}$) | n = 7 ($10^{-1}$) | n = 8 ($10^0$) |
| Reactivity [m] | VF | | | | | | | | |
| | F | | | | | | | | |
| | M | | | | | | | | |
| | S | | | | | | | | |
| | P | | | | | | | | |
| | MA | | | | | | | | |
| | R | | | | | | | | GLY |

## Section S3. Gas oxidation mechanism

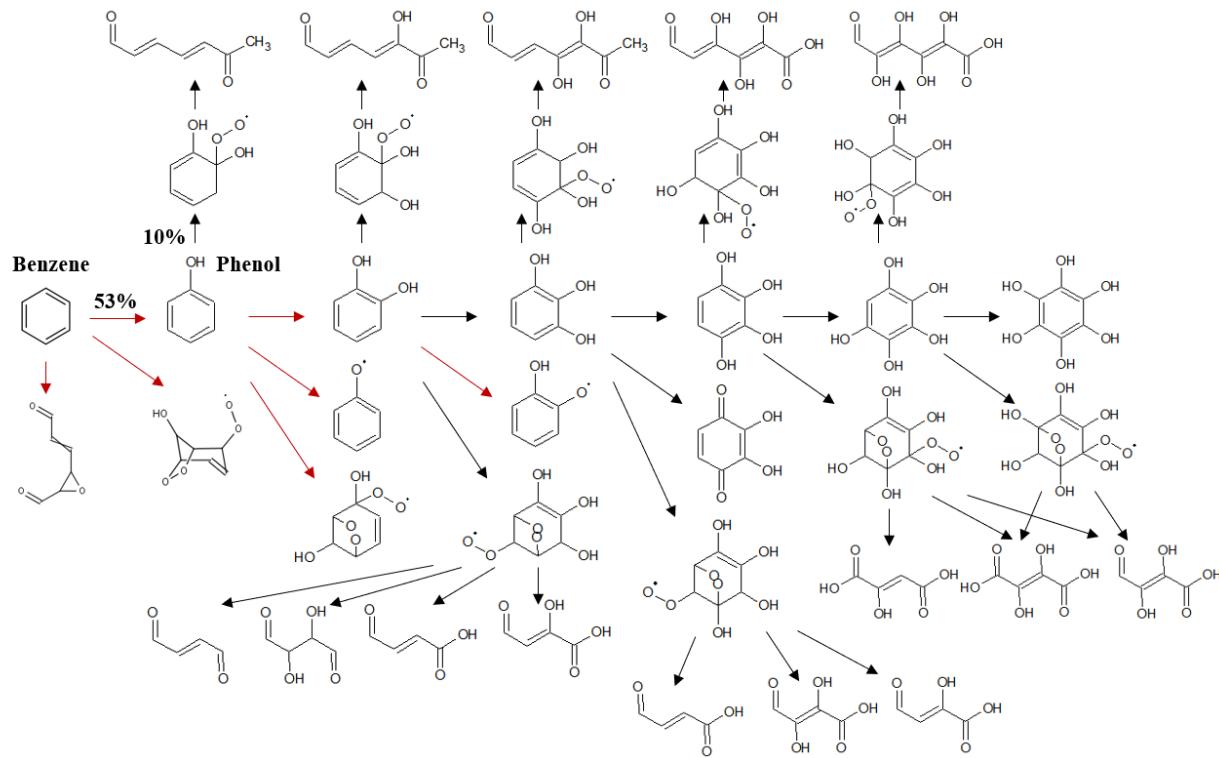



**Figure S2.** The benzene and phenol oxidation mechanisms to form low volatility products originating from multi-hydroxybenzenes.

## Section S4. The mechanisms to produce a phenoxy radical in aqueous aerosol

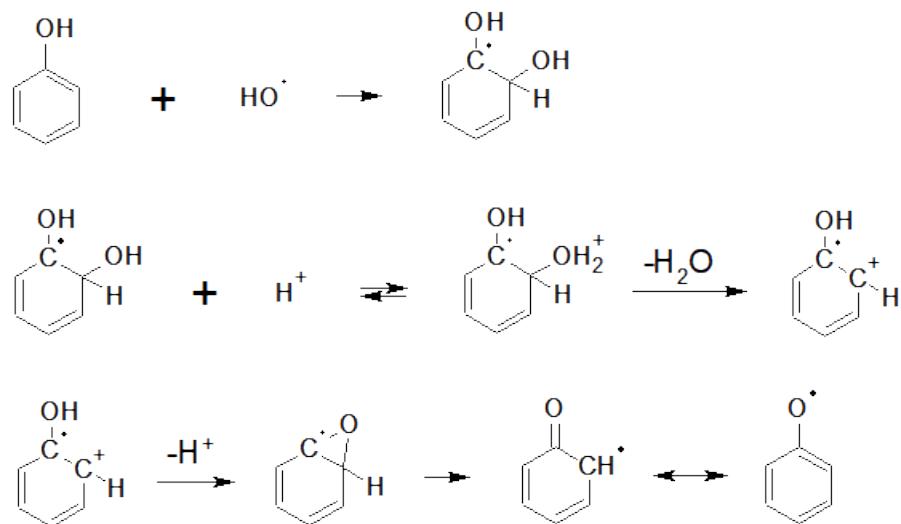



Figure S3. The scheme of phenol oxidation path to form phenoxy radicals in aqueous phase.

## OH radical formation in aqueous aerosol

The radical species produced in gas phase and ozone can be partitioned to aqueous phase. $K_p$ denotes the gas-particle partitioning constant and $K_a$, the acid dissociation constant. Additionally, radicals can be produced via the photolysis of H2O2 and HONO, or aqueous phase reaction (Liang and Jacobson, 1999). $kaq$ denotes the reaction rate constant of a radical in aqueous phase and kph, the photolysis rate constant of chemical species. Term $V = NA \times V(aq)$, where Na $(6.022 \times 1023$ molecule mol-1) is the Avogadro constant and V(aq) (L cm-3) is the volume concentration of inorganic salt seeded aqueous phase in the air.

$$OH\ (g) \leftrightarrow OH\ (aq) \qquad K_{p,OH} = 4.58 \times 10^{-20} \exp(5250/T) \times T/(V(aq)\rho in) \qquad (R1)$$

(Hanson et al., 1992; Jacob, 1986)

$$HO_2\ (g) \leftrightarrow HO_2\ (aq) \qquad K_{p,HO_2} = 3.95 \times 10^{-20} \exp(6600/T) \times T/(V(aq)\rho in) \qquad (R2)$$

(Hanson et al., 1992; Jacob, 1986)

$$O_3\ (g) \leftrightarrow O_3\ (aq) \qquad K_{p,O_3} = 3.07 \times 10\text{-}19 \exp(2380/T) \times T/(V(aq)\rho in) \qquad (R3)$$

(Chameides, 1984; Jacob, 1986)

$$HO_2\ (aq) \leftrightarrow O_2^- + H^+ \qquad K_{a,HO_2} = 1.17 \times 10^{-3} \exp(-1046.4/T) \qquad (R4)$$

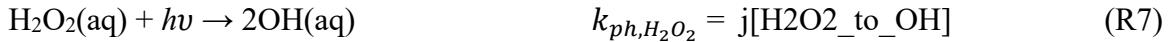
(Bielski et al., 1985)

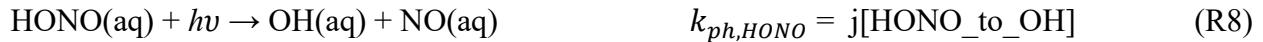
$$HO_2\ (aq) + HO_2\ (aq) \rightarrow H_2O_2\ (aq) + O_2\ (aq) \qquad k_{aq,S5} = 7.14 \times 10^9 \exp(-2700/T)/V \qquad (R5)$$

(Bielski et al., 1985)

$$O_2^- + O_3(aq) \rightarrow OH(aq) + OH^- + 2O_2(aq) \qquad k_{aq,S6} = 2.30 \times 10^{11} \exp(-1500/T)/V \qquad (R6)$$

(Sehested et al., 1983; Bielski et al., 1985)

$$H_2O_2(aq) + h\upsilon \rightarrow 2OH(aq) \qquad k_{ph,H_2O_2} = j[H2O2\_to\_OH] \qquad (R7)$$

(Lin et al., 1978; Molina and Molina, 1981; Nicovich and Wine, 1988)

$$HONO(aq) + h\upsilon \rightarrow OH(aq) + NO(aq) \qquad k_{ph,HONO} = j[HONO\_to\_OH] \qquad (R8)$$

(Bongartz et al., 1991; Atkinson et al., 1997)

**Phenoxy radical formation via the reaction with an OH radical in aqueous aerosol**

$$C_6H_5OH\ (g) \rightarrow C_6H_5OH\ (aq) \qquad K_p = 2.89 \times 10^{-5} \qquad (R9)$$

(Dohnal and Fenclova, 1995; Abd-El-Bary et al., 1986)

$$OH\ (aq) + C_6H_5OH\ (aq) \rightarrow HO\text{-}C_6H_5{}^\bullet OH\ (aq) \qquad k_{aq,S10} = 6.6 \times 10^9\ M^{-1}\ s^{-1} \qquad (R10)$$

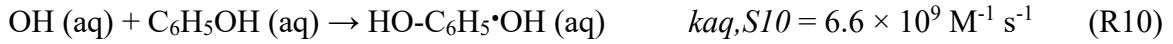
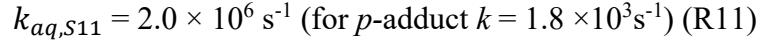
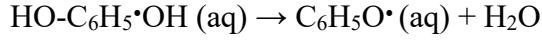
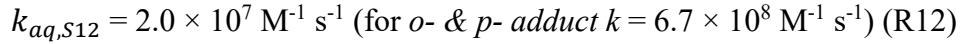
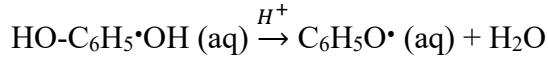
(Ross et al., 1998)

$$HO\text{-}C_6H_5{}^\bullet OH\ (aq) \rightarrow C_6H_5O^\bullet\ (aq) + H_2O$$

$$k_{aq,S11} = 2.0 \times 10^6\ s^{-1}\ (\text{for } p\text{-adduct } k = 1.8 \times 10^3 s^{-1}) \quad (R11)$$

(Mvula et al., 2001; Das, 2005)

$$HO\text{-}C_6H_5{}^\bullet OH\ (aq) \xrightarrow{H^+} C_6H_5O^\bullet\ (aq) + H_2O$$

$$k_{aq,S12} = 2.0 \times 10^7\ M^{-1}\ s^{-1}\ (\text{for } o\text{- \& } p\text{- adduct } k = 6.7 \times 10^8\ M^{-1}\ s^{-1}) \quad (R12)$$

(Mvula et al., 2001; Das, 2005)

**Phenoxy radical formation via irradiation under UV light**

$$AroH \xrightarrow{h\upsilon} Ar^{\bullet+}OH - e^- \qquad\qquad (R13)$$

(Siano et al., 2020)

$$Ar^{\bullet+}OH \xrightarrow{k_H} ArO^\bullet + H^+ \qquad\qquad (R14)$$

(Dixon and Murphy, 1976; Siano et al., 2020)

# References

Abd-El-Bary, M. F., Hamoda, M. F., Tanisho, S., and Wakao, N.: Henry's constants for phenol over its diluted aqueous solution, Journal of Chemical and Engineering Data, 31, 229-230, 1986.

Atkinson, R., Baulch, D., Cox, R., Hampson Jr, R., Kerr, J., Rossi, M., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry: supplement VI. IUPAC subcommittee on gas kinetic data evaluation for atmospheric chemistry, Journal of Physical and Chemical Reference Data, 26, 1329-1499, 1997.

Beardsley, R., Jang, M., Ori, B., Im, Y., Delcomyn, C. A., and Witherspoon, N.: Role of sea salt aerosols in the formation of aromatic secondary organic aerosol: yields and hygroscopic properties, Environmental Chemistry, 10, 167-177, 2013.

Beardsley, R. L. and Jang, M.: Simulating the SOA formation of isoprene from partitioning and aerosol phase reactions in the presence of inorganics, Atmospheric Chemistry and Physics, 16, 5993-6009, 2016.

Bielski, B. H., Cabelli, D. E., Arudi, R. L., and Ross, A. B.: Reactivity of HO2/O− 2 radicals in aqueous solution, Journal of physical and chemical reference data, 14, 1041-1100, 1985.

Bongartz, A., Kames, J., Welter, F., and Schurath, U.: Near-UV absorption cross sections and trans/cis equilibrium of nitrous acid, The Journal of Physical Chemistry, 95, 1076-1082, 1991.

Borrás, E. and Tortajada-Genaro, L. A.: Secondary organic aerosol formation from the photo-oxidation of benzene, Atmospheric Environment, 47, 154-163, 2012.

Cao, G. and Jang, M.: An SOA model for toluene oxidation in the presence of inorganic aerosols, Environmental science & technology, 44, 727-733, 2010.

Chameides, W. L.: The photochemistry of a remote marine stratiform cloud, Journal of Geophysical Research: Atmospheres, 89, 4739-4755, 1984.

Das, T. N.: Oxidation of phenol in aqueous acid: Characterization and reactions of radical cations vis-à-vis the phenoxyl radical, The Journal of Physical Chemistry A, 109, 3344-3351, 2005.

Dixon, W. T. and Murphy, D.: Determination of the acidity constants of some phenol radical cations by means of electron spin resonance, Journal of the Chemical Society, Faraday Transactions 2: Molecular and Chemical Physics, 72, 1221-1230, 1976.

Dohnal, V. and Fenclova, D.: Air-water partitioning and aqueous solubility of phenols, Journal of Chemical and Engineering Data, 40, 478-483, 1995.

Han, S. and Jang, M.: Prediction of secondary organic aerosol from the multiphase reaction of gasoline vapor by using volatility–reactivity base lumping, Atmospheric Chemistry and Physics, 22, 625-639, 2022.

Hanson, D. R., Burkholder, J. B., Howard, C. J., and Ravishankara, A.: Measurement of hydroxyl and hydroperoxy radical uptake coefficients on water and sulfuric acid surfaces, The Journal of Physical Chemistry, 96, 4979-4985, 1992.

Im, Y., Jang, M., and Beardsley, R.: Simulation of aromatic SOA formation using the lumping model integrated with explicit gas-phase kinetic mechanisms and aerosol-phase reactions, Atmospheric Chemistry and Physics, 14, 4013-4027, 2014.

Jacob, D. J.: Chemistry of OH in remote clouds and its role in the production of formic acid and peroxymonosulfate, Journal of Geophysical Research: Atmospheres, 91, 9807-9826, 1986.

Jang, M., Czoschke, N. M., and Northcross, A. L.: Semiempirical model for organic aerosol growth by acid-catalyzed heterogeneous reactions of organic carbonyls, Environmental science & technology, 39, 164-174, 2005.

Jang, M., Czoschke, N. M., Lee, S., and Kamens, R. M.: Heterogeneous atmospheric aerosol production by acid-catalyzed particle-phase reactions, Science, 298, 814-817, 2002.

Jenkin, M., Saunders, S., Wagner, V., and Pilling, M.: Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part B): tropospheric degradation of aromatic volatile organic compounds, Atmospheric Chemistry and Physics, 3, 181-193, 2003.

Jenkin, M. E., Saunders, S. M., and Pilling, M. J.: The tropospheric degradation of volatile organic compounds: a protocol for mechanism development, Atmospheric Environment, 31, 81-104, 1997.

Kleindienst, A. and Bullock, M. R.: A critical analysis of the role of the neurotrophic protein S100B in acute brain injury, Journal of neurotrauma, 23, 1185-1200, 2006.

Liang, J. and Jacobson, M. Z.: A study of sulfur dioxide oxidation pathways over a range of liquid water contents, pH values, and temperatures, Journal of Geophysical Research: Atmospheres, 104, 13749-13769, 1999.

Lin, C., Rohatgi, N., and DeMore, W.: Ultraviolet absorption cross sections of hydrogen peroxide, Geophysical Research Letters, 5, 113-115, 1978.

Molina, L. T. and Molina, M. J.: UV absorption cross sections of HO2NO2 vapor, Journal of Photochemistry, 15, 97-108, 1981.

Mvula, E., Schuchmann, M. N., and von Sonntag, C.: Reactions of phenol-OH-adduct radicals. Phenoxyl radical formation by water elimination vs. oxidation by dioxygen, Journal of the Chemical Society, Perkin Transactions 2, 264-268, 2001.

Nakao, S., Clark, C., Tang, P., Sato, K., and Cocker Iii, D.: Secondary organic aerosol formation from phenolic compounds in the absence of NO x, Atmospheric Chemistry and Physics, 11, 10649-10660, 2011.

Nakao, S., Tang, P., Tang, X., Clark, C. H., Qi, L., Seo, E., Asa-Awuku, A., and Cocker III, D.: Density and elemental ratios of secondary organic aerosol: Application of a density prediction method, Atmospheric Environment, 68, 273-277, 2013.

Ng, N., Kroll, J., Chan, A., Chhabra, P., Flagan, R., and Seinfeld, J.: Secondary organic aerosol formation from m-xylene, toluene, and benzene, Atmospheric Chemistry and Physics, 7, 3909-3922, 2007.

Nicovich, J. and Wine, P.: Temperature-dependent absorption cross sections for hydrogen peroxide vapor, Journal of Geophysical Research: Atmospheres, 93, 2417-2421, 1988.

Odian, G.: Principles of polymerization, John Wiley & Sons2004.

Pankow, J. F.: An absorption model of gas/particle partitioning of organic compounds in the atmosphere, Atmospheric Environment, 28, 185-188, 1994.

Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P.: Numerical Recipes in Fortran 90: Numerical recipes in Fortran 77V. 2. Numerical recipes in Fortran 90, Cambridge University Press1996.

Ross, A., Mallard, W., Helman, W., Buxton, G., Huie, R., and Neta, P.: NDRL-NIST Solution Kinetics Database: Ver. 3, Notre Dame Radiation Laboratory, Notre Dame, IN and NIST Standard Reference Data, Gaithersburg, MD, 1998.

Saunders, S. M., Jenkin, M. E., Derwent, R., and Pilling, M.: Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part A): tropospheric degradation of non-aromatic volatile organic compounds, Atmospheric Chemistry and Physics, 3, 161-180, 2003.

Schell, B., Ackermann, I. J., Hass, H., Binkowski, F. S., and Ebel, A.: Modeling the formation of secondary organic aerosol within a comprehensive air quality model system, Journal of Geophysical Research: Atmospheres, 106, 28275-28293, 2001.

Sehested, K., Holcman, J., and Hart, E. J.: Rate constants and products of the reactions of e-aq, dioxide (1-)(O2-) and proton with ozone in aqueous solutions, The Journal of Physical Chemistry, 87, 1951-1954, 1983.

Siano, G., Crespi, S., and Bonesi, S. M.: Direct Irradiation of Phenol and Para-Substituted Phenols with a Laser Pulse (266 nm) in Homogeneous and Micro-heterogeneous Media. A Time-Resolved Spectroscopy Study, The Journal of Organic Chemistry, 85, 14012-14025, 2020.

Yee, L., Kautzman, K., Loza, C., Schilling, K., Coggon, M., Chhabra, P., Chan, M., Chan, A., Hersey, S., and Crounse, J.: Secondary organic aerosol formation from biomass burning intermediates: phenol and methoxyphenols, Atmospheric Chemistry and Physics, 13, 8019-8043, 2013.

Yu, Z., Jang, M., and Madhu, A.: Prediction of Phase State of Secondary Organic Aerosol Internally Mixed with Aqueous Inorganic Salts, The Journal of Physical Chemistry A, 125, 10198-10206, 2021.

Zhao, L., Li, P., and Yalkowsky, S. H.: Predicting the entropy of boiling for organic compounds, Journal of chemical information and computer sciences, 39, 1112-1116, 1999.

Zhou, C., Jang, M., and Yu, Z.: Simulation of SOA formation from the photooxidation of monoalkylbenzenes in the presence of aqueous aerosols containing electrolytes under various NO x levels, Atmospheric Chemistry and Physics, 19, 5719-5735, 2019.

Zuend, A., Marcolli, C., Booth, A., Lienhard, D. M., Soonsin, V., Krieger, U., Topping, D. O., McFiggans, G., Peter, T., and Seinfeld, J. H.: New and extended parameterization of the thermodynamic model AIOMFAC: calculation of activity coefficients for organic-inorganic mixtures containing carboxyl, hydroxyl, carbonyl, ether, ester, alkenyl, alkyl, and aromatic functional groups, Atmospheric Chemistry and Physics, 11, 9155-9206, 2011.