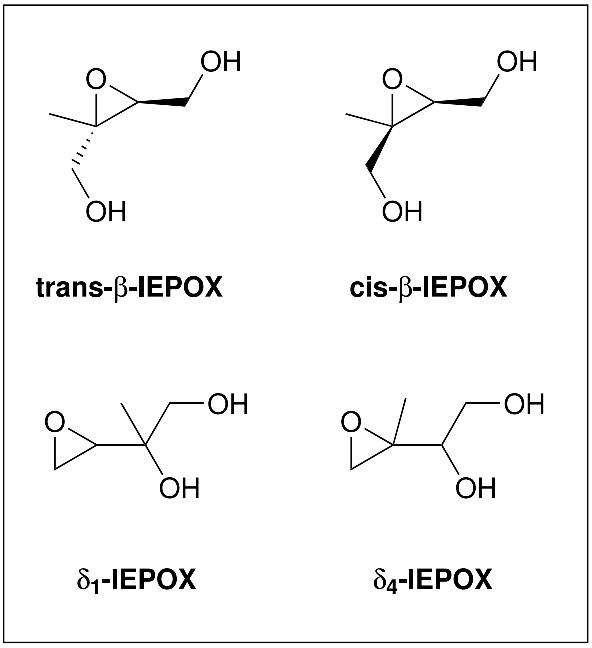


Figure S1: The isomers of IEPOX.

## S1 Density calculation

COSMO*therm* estimates the density of a pure liquid using its corrected molar liquid volume $\widetilde{V}_i$:

$$\rho_i = \frac{MW_i}{\widetilde{V}_i(T) \cdot N_A}, \tag{S1}$$

where $N_A$ is the Avogadro constant. The temperature dependent volume $\widetilde{V}_i$ is calculated from a quantitative-structure-property-relationship (QSPR):

$$\begin{aligned}\widetilde{V}_i(T) = c_1^T(T/T_{\text{room}} - 1) + c_2^T(T/T_{\text{room}} - 1)^2\widetilde{V}_i(T_{\text{room}}) + \\ c^T_{V_{\text{COSMO}}} V_i^{\text{COSMO}} + c^T_{M_2} M_{2_i} + c^T_{M_2^2} M_{2_i}^2 + c^T_{N_{\text{ring}}} N_i^{\text{ring}} + \\ c^T_{V_{C1}}(T/T_{\text{room}} - 1)V_i^{\text{COSMO}} + c^T_{V_{C2}} * (T/T_{\text{room}} - 1)^2 V_i^{\text{COSMO}} + \\ \sum_k^{elements} c^T_{A_k} A_i^k + c_0^T,\end{aligned} \tag{S2}$$

where

$$\widetilde{V}_i(T_{\mathrm{room}}) = c_{V_{\mathrm{COSMO}}} V_i^{\mathrm{COSMO}} + c_{M_2} M_{2_i} + c_{M_2^2} M_{2_i}^2 + c_{N_{\mathrm{ring}}} N_i^{\mathrm{ring}} + \sum_{k}^{elements} c_{A_k} A_i^k + c_0, \quad \text{(S3)}$$

$M$ is the second $\sigma$-moment of the compound, $A_i^k$ is the area of surface if each atom $k$, $N_{\mathrm{ring}}$ is the number of ring atoms in the compound and $c$ are parameters of the QSPR calculation.

For a mixture of multiple compounds, the density is calculated using the molar mass and the volume of the solution, $MW_{\mathrm{solution}}$ and $\widetilde{V}_{\mathrm{solution}}$ respectively. Both are calculated as the weighted averages of the individual compounds in the solution:

$$MW_{\mathrm{solution}} = \sum_i x_i MW_i \quad \text{(S4)}$$

$$\widetilde{V}_{\mathrm{solution}}(T) = \sum_i x_i \widetilde{V}_i(T) \quad \text{(S5)}$$

where $x_i$ is the mole fraction of compound $i$.

## S2 Ions in COSMO*therm*

When salts are included in a system, COSMO*therm* treats the ions of the salt as separate entities and gives the mole fractions of each ion and neutral compound as normalized to one (for example in a binary mixture with water, $x'_{\mathrm{H_2O}} + x'_{\mathrm{M^+}} + x'_{\mathrm{X^-}} = 1$). On the other hand, in experiments the salt is considered as a single compound ($x_{\mathrm{H_2O}} + x_{\mathrm{MX}} = 1$). This creates a difference between the calculation and the experimental framework for expressing non-measurable properties, such as activity coefficients, while keeping the activity in both frameworks equal. For example, the activity of compound $i$ can equally be expressed using either the activity coefficient of the experimental ($\gamma$) or the calculation ($\gamma'$) framework:

$$a_i = x_i \gamma_i = x'_i \gamma'_i \quad \text{(S6)}$$

The mole fraction in the experimental framework can be expressed using the calculation framework of COSMO*therm*:

$$x_i = \frac{x'_i}{1 - x'_{\mathrm{M}^+}} \tag{S7}$$

assuming that the stoichiometry of the anion is 1 and of the cation is higher than or equal to 1. Combining Equations S6 and S7 allows us to calculate the activity coefficient in the experimental framework:

$$\gamma_i = \frac{x'_i}{x_i}\gamma'_i = (1 - x'_{\mathrm{M}^+})\gamma'_i \tag{S8}$$

Calculating solubilities as mole fractions, the different frame works have to be considered for both the solubility value and the mole fraction of the salt in the solvent. In calculating the solubility of a salt, COSMO*therm* allows for the definition of the solute as one salt entity, giving the result in the experimental framework. Figure S3 illustrates a ternary system (solvent containing one salt and one neutral compound) at the solubility limit using the mole fractions given by COSMO*therm* ($x'$) to express the mole fraction of each component in the system. The solubility (in mole fraction) can be re-scaled to the experimental framework by dividing with the new size of the system:

$$x_{\mathrm{SOL}} = \frac{x'_{\mathrm{SOL}}}{1 - (1 - x'_{\mathrm{SOL}}) \cdot x'_{\mathrm{M}^+}} \tag{S9}$$

Note that here $x'_{\mathrm{M}^+}$ is the mole fraction of the cation in the solvent as opposed to the whole solution, as in Equation (S8). Similarly, the mole fraction of salt in the solvent has to be calculated taking into account the new size of the solvent (again assuming that in the salt $\mathrm{M}_{\nu^+}\mathrm{X}_{\nu^-}$, $\nu^- = 1$ and $\nu^+ \geq \nu^-$):

$$x_{\mathrm{MX}} = \frac{x'_{\mathrm{X}^-}}{1 - x'_{\mathrm{M}^+}} \tag{S10}$$

Toure et al.[S1–S3] have studied the effect of hydrating strongly polar metallic mono-atomic ions in COSMO*therm* calculations. To use an appropriate hydration number for the sodium cation, we tested the effect of the number of water molecules on the relative solubilities of

$\alpha$-pinene-OS-1 in aqueous ammonium sulfate solutions. Considering the water molecules attached to the hydrated sodium ion of the solute ($Na \cdot kH_2O$) as part of the solvent, the mole fraction of the inorganic salt (MX) in the solvent needs to be calculated for each solubility value. Since the mole fraction of $H_2O$ in the solvent changes by the addition of water molecules of the hydrated sodium ions, the mole fraction of the inorganic salt has to be scaled with the new solvent. The amount of solvent in the system at the solubility limit is originally $1 - x_{\mathrm{SOL}}$, and the additional water from the hydrated solute ($k \cdot x_{\mathrm{SOL}}$) is added to the original solvent ($1 - x_{\mathrm{SOL}} + k \cdot x_{\mathrm{SOL}}$). This is then used to divide the amount of inorganic salt.

$$x_{\mathrm{MX,dry}} = \frac{x_{\mathrm{MX}}(1 - x_{\mathrm{SOL}})}{1 + (k-1) \cdot x_{\mathrm{SOL}}} \tag{S11}$$

The solubility used to calculate the mole fraction of inorganic salt in the solvent is the SLE solubility in 0.09 mole fraction of the inorganic salt scaled by the relative solubility from the relative screening calculation. All of the solubilities at this point are calculated using the hydrated sodium ion. Some of the relative solubilities are above one at low inorganic salt mole fractions, which leads to negative values for $x_{\mathrm{MX}}$ from Equation S11. In these cases, the value of $x_{\mathrm{MX}}$ is set to 0.

In addition, the solubility needs to be re-calculated taking into account the increase in the mole fraction of the solvent caused by the dissociation of the hydrated solute ($NaOS \cdot kH_2O$). The final amount of solvent and solute in the system is the original 1 mole and an additional $k \cdot x_{\mathrm{SOL}}$ of water:

$$x_{\mathrm{SOL,dry}} = \frac{x_{\mathrm{SOL}}}{1 + k \cdot x_{\mathrm{SOL}}}, \tag{S12}$$

Using Equations S10 and S12, we obtain the relative solubilities seen in Figure S2. The mole fractions of the inorganic salt have not been re-scaled, since we only have the relative solubilities of the different hydrates, not the absolute solubilities. With a dry sodium cation ($k = 0$), COSMO*therm* predicts strong salting-in behavior at low ammonium sulfate concentrations. At $k = 4$, COSMO*therm* predicts salting-out through the whole ammonium sulfate concentration range and after $k = 5$ the relative solubility result has converged. We are using this fully hydrated sodium cation in our solubility calculations.

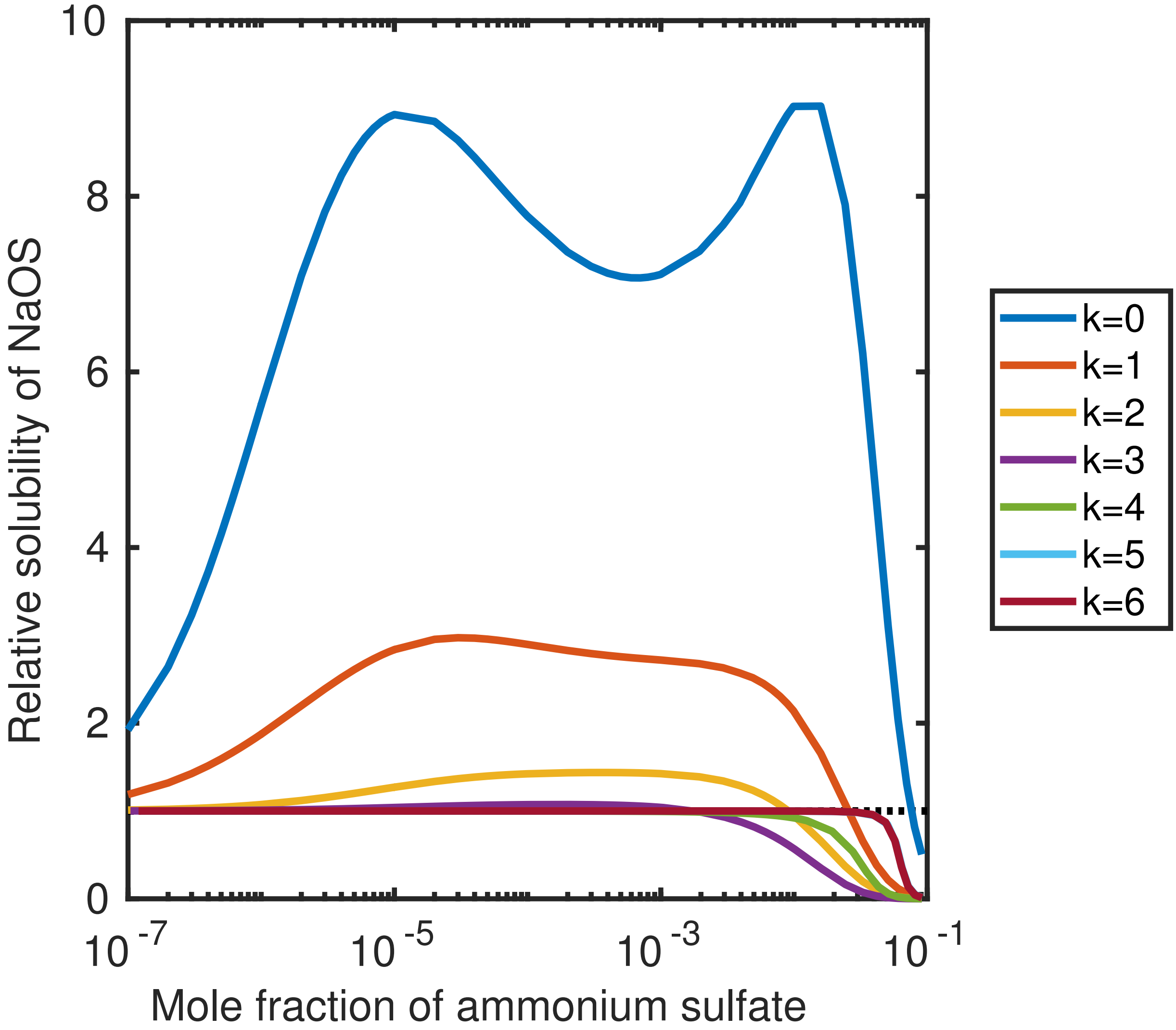


Figure S2: The relative solubilities ($x_{\mathrm{SOL}} = 1$ in pure water) of the sodium salt of $\alpha$-pinene-OS-1 $(NH_4)_2SO_4$ (aq) solutions ($T$ = 298.15 K) estimated using the relative screening in COSMO*therm*. The hydrated sodium cation contains $k$ water molecules.

For the $k = 5$, the absolute solubilities of the hydrated NaOS salts were calculated using the SLE solubilities in 0.09 mole fraction of each inorganic salt (AS and ABS) as a reference. Those solubility values were then used to calculate the corrected mole fraction of the inorganic salt for each of the organosulfate solutes. In Figure S5 the range of the ammonium sulfate varies depending on the absolute solubility of the solute, where the higher absolute solubility leads to a smaller mole fraction of the inorganic salt in the solvent.

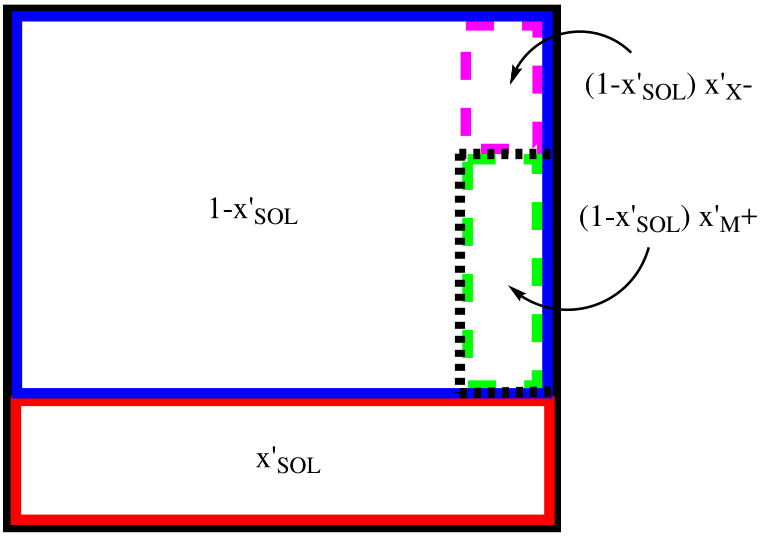


Figure S3: A ternary system at the solubility limit showing the mole fraction of each component in the system using the mole fractions given by COSMO*therm* for the solubility and the mole fractions of the salt ions in the solvent. Color coding: red = solute, blue = solvent, magenta = anion, green = cation.

**Table S1: $pK_a$ values of the organosulfates and sulfuric acid in water, at 298.15 K, estimated using COSMO*therm*. Literature values for methyl bisulfate -2.6 and for sulfuric acid -3.0 calculated by extrapolation. The solubilities ($x_{SOL}$) were calculated using the SLE solver and only conformers containing 0 intramolecular H-bonds. The dissociation corrected solubility ($x^{DC}$) was then calculated using Equation (11). For all of the compounds, the dissociation correction is approximate, as Equation (11) gives values >1.**

| | $pK_a$ | $x_{SOL}$ | $x^{DC}$ | $x_{MX}$ |
|---|---|---|---|---|
| $\alpha$-pinene-OS-1 | -3.19 | $1.03 \cdot 10^{-3}$ | 1.00 | $6.63 \cdot 10^{-2}$ |
| $\alpha$-pinene-OS-2 | -3.19 | $3.69 \cdot 10^{-3}$ | 1.00 | $6.19 \cdot 10^{-2}$ |
| $\alpha$-pinene-OS-3 | -2.42 | $4.64 \cdot 10^{-3}$ | 1.00 | - |
| $\alpha$-pinene-OS-4 | -3.12 | $2.60 \cdot 10^{-3}$ | 1.00 | - |
| $\alpha$-pinene-OS-5 | -4.23 | $6.72 \cdot 10^{-3}$ | 1.00 | - |
| $\alpha$-pinene-OS-6 | -4.58 | $6.93 \cdot 10^{-3}$ | 1.00 | - |
| $\beta$-pinene-OS-1 | -4.24 | $1.72 \cdot 10^{-3}$ | 1.00 | $6.45 \cdot 10^{-2}$ |
| $\beta$-pinene-OS-2 | -2.98 | $3.05 \cdot 10^{-3}$ | 1.00 | $6.88 \cdot 10^{-2}$ |
| limonene-OS-1 | -3.00 | $2.52 \cdot 10^{-3}$ | 1.00 | $6.56 \cdot 10^{-2}$ |
| limonene-OS-2 | -2.90 | $1.92 \cdot 10^{-3}$ | 1.00 | $6.07 \cdot 10^{-2}$ |
| limonene-OS-3 | -3.17 | $1.16 \cdot 10^{-3}$ | 1.00 | - |
| limonene-OS-4 | -3.64 | $1.48 \cdot 10^{-3}$ | 1.00 | - |
| isoprene-OS-1 | -3.87 | - | - | - |
| isoprene-OS-2 | -4.49 | - | - | - |
| isoprene-OS-3 | -3.94 | - | - | - |
| isoprene-OS-4 | -2.37 | - | - | - |
| Methyl bisulfate | -4.03 | - | - | - |
| Sulfuric acid | -3.51 | - | - | - |

**Table S2: LLE solubilities of the OS, AS and ABS, and SLE solubilities of NaOS. OS = organosulfate, NaOS = sodium salt of the organosulfate, AS = 0.09 mole fraction aqueous solution of ammonium sulfate, ABS = 0.09 mole fraction aqueous solution of ammonium bisulfate. Note that the actual concentration of the inorganic salt in the NaOS systems varies based on the solubility according to Equation S11.**

| Solvent | AS | | ABS | | OS | |
|---|---|---|---|---|---|---|
| Solute | OS | NaOS | OS | NaOS | AS | ABS |
| $\alpha$-pinene-OS-1 | $8.73{\cdot}10^{-7}$ | $1.24{\cdot}10^{-3}$ | $5.37{\cdot}10^{-5}$ | $3.82{\cdot}10^{-2}$ | 0.973 | 0.884 |
| $\alpha$-pinene-OS-2 | $4.52{\cdot}10^{-6}$ | $1.21{\cdot}10^{-3}$ | $2.78{\cdot}10^{-4}$ | $3.52{\cdot}10^{-2}$ | 0.942 | 0.729 |
| $\alpha$-pinene-OS-3 | $7.92{\cdot}10^{-6}$ | $2.36{\cdot}10^{-3}$ | $4.43{\cdot}10^{-4}$ | $4.69{\cdot}10^{-2}$ | 0.677 | 0.493 |
| $\alpha$-pinene-OS-4 | $2.58{\cdot}10^{-6}$ | $1.64{\cdot}10^{-3}$ | $2.17{\cdot}10^{-4}$ | $3.92{\cdot}10^{-2}$ | 0.830 | 0.670 |
| $\alpha$-pinene-OS-5 | $1.56{\cdot}10^{-5}$ | $6.08{\cdot}10^{-3}$ | $5.32{\cdot}10^{-4}$ | $5.65{\cdot}10^{-2}$ | 0.694 | 0.546 |
| $\alpha$-pinene-OS-6 | $1.87{\cdot}10^{-5}$ | $4.82{\cdot}10^{-3}$ | $6.07{\cdot}10^{-4}$ | $5.11{\cdot}10^{-2}$ | 0.614 | 0.478 |
| $\beta$-pinene-OS-1 | $1.40{\cdot}10^{-6}$ | $1.09{\cdot}10^{-3}$ | $8.77{\cdot}10^{-5}$ | $3.66{\cdot}10^{-2}$ | 0.984 | 0.890 |
| $\beta$-pinene-OS-2 | $4.50{\cdot}10^{-6}$ | $2.13{\cdot}10^{-3}$ | $2.69{\cdot}10^{-4}$ | $4.66{\cdot}10^{-2}$ | 0.875 | 0.657 |
| limonene-OS-1 | $2.04{\cdot}10^{-6}$ | $1.20{\cdot}10^{-3}$ | $1.60{\cdot}10^{-4}$ | $3.93{\cdot}10^{-2}$ | 0.935 | 0.742 |
| limonene-OS-2 | $1.38{\cdot}10^{-6}$ | $8.07{\cdot}10^{-4}$ | $1.12{\cdot}10^{-4}$ | $3.05{\cdot}10^{-2}$ | 0.945 | 0.737 |
| limonene-OS-3 | $6.84{\cdot}10^{-7}$ | $1.54{\cdot}10^{-3}$ | $5.86{\cdot}10^{-5}$ | $4.50{\cdot}10^{-2}$ | 0.980 | 0.852 |
| limonene-OS-4 | $1.23{\cdot}10^{-6}$ | $1.71{\cdot}10^{-3}$ | $1.00{\cdot}10^{-4}$ | $4.83{\cdot}10^{-2}$ | 0.928 | 0.725 |
| isoprene-OS-1 | $1.03{\cdot}10^{-3}$ | $1.42{\cdot}10^{-2}$ | $9.78{\cdot}10^{-3}$ | $5.40{\cdot}10^{-2}$ | 0.546 | 0.396 |
| isoprene-OS-2 | $1.04{\cdot}10^{-3}$ | $9.09{\cdot}10^{-3}$ | $9.61{\cdot}10^{-3}$ | $4.95{\cdot}10^{-2}$ | 0.481 | 0.344 |
| isoprene-OS-3 | $3.20{\cdot}10^{-3}$ | $1.60{\cdot}10^{-2}$ | $4.83{\cdot}10^{-2}$ | $5.63{\cdot}10^{-2}$ | 0.440 | 0.125 |
| isoprene-OS-4 | $2.95{\cdot}10^{-3}$ | $1.04{\cdot}10^{-2}$ | $5.87{\cdot}10^{-2}$ | $5.02{\cdot}10^{-2}$ | 0.593 | 0.179 |
| Cis-$\beta$-IEPOX | $6.43{\cdot}10^{-3}$ | - | - | - | 0.900 | - |
| Trans-$\beta$-IEPOX | $6.34{\cdot}10^{-3}$ | - | - | - | 0.905 | - |
| $\delta_1$-IEPOX | $1.57{\cdot}10^{-2}$ | - | - | - | 0.903 | - |
| $\delta_4$-IEPOX | $6.71{\cdot}10^{-3}$ | - | - | - | 0.912 | - |
| Methyl bisulfate | $1.91{\cdot}10^{-2}$ | $3.02{\cdot}10^{-2}$ | $5.62{\cdot}10^{-2}$ | $5.64{\cdot}10^{-2}$ | 0.441 | 0.320 |

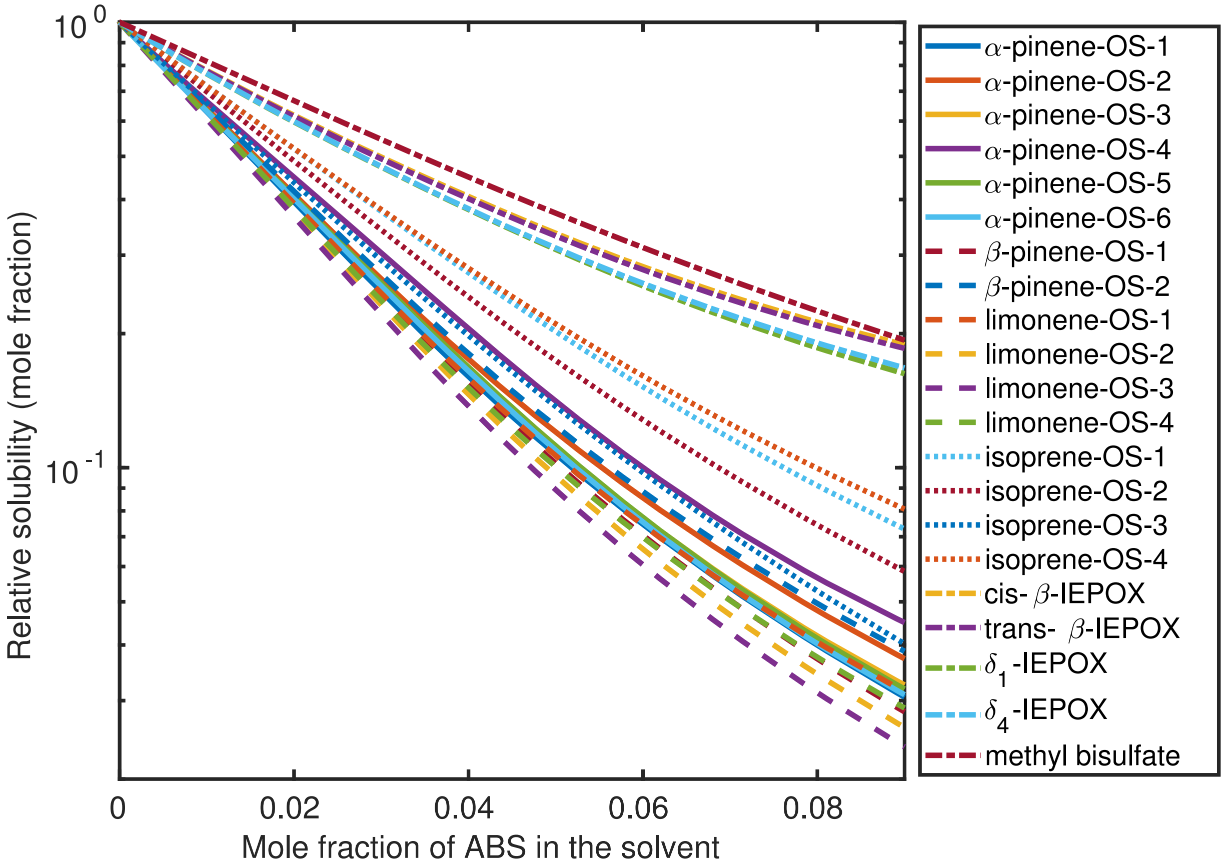


Figure S4: The relative solubilities of organosulfates in $NH_4HSO_4$ (aq) solutions ($T = 298.15$ K) estimated using the relative screening in COSMO*therm*.

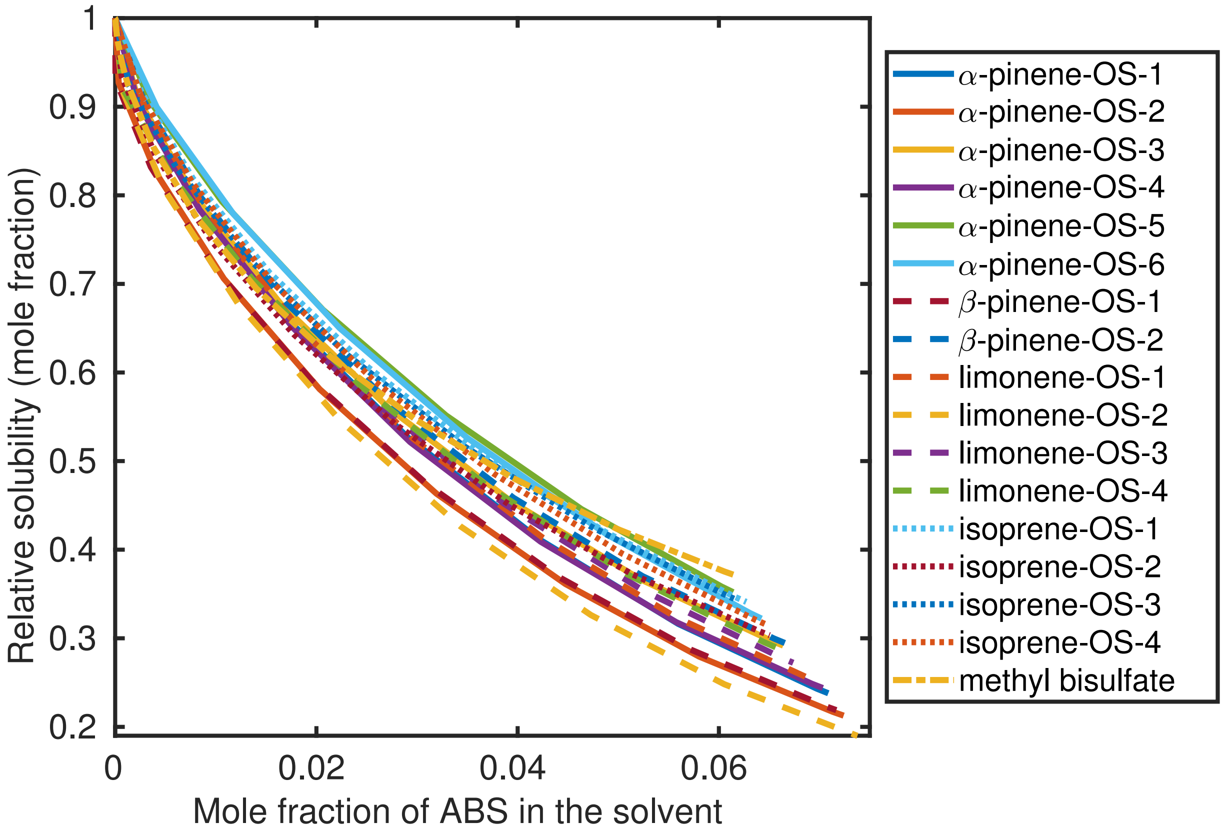


Figure S5: The relative solubilities of sodium salts of the organosulfates in $NH_4HSO_4$ (aq) solutions ($T$ = 298.15 K) estimated using the relative screening in COSMO*therm*.

**Table S3: Activity coefficients of the organics and water in stable binary solutions, at 298.15 K.**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^I$(org) | $\ln \gamma^I(H_2O)$ |
|---|---|---|---|
| | α-pinene-OS-1 | | |
| 1.00E-08 | 1 | 6.24734649 | 0.00000007 |
| 2.06E-04 | 0.9998 | 6.22811677 | 0.00000205 |
| 4.12E-04 | 0.9996 | 6.20896327 | 0.00000798 |
| 6.17E-04 | 0.9994 | 6.18988691 | 0.00001782 |
| 8.23E-04 | 0.9992 | 6.17088756 | 0.00003155 |
| 1.03E-03 | 0.999 | 6.15196503 | 0.00004913 |
| 0.4825 | 0.5175 | 0.00161722 | 0.65774678 |

**Table S3 – continued from previous page**

| $x$(org) | $x$($H_2O$) | $\ln \gamma^{I}$(org) | $\ln \gamma^{I}$($H_2O$) |
|---|---|---|---|
| 0.586 | 0.414 | -0.01961669 | 0.67911130 |
| 0.6895 | 0.3105 | -0.01786611 | 0.67203684 |
| 0.793 | 0.207 | -0.01199478 | 0.64732295 |
| 0.8965 | 0.1035 | -0.00436202 | 0.58261809 |
| 1 | 1.00E-08 | 0.00000000 | 0.40639492 |
| | | $\alpha$-pinene-OS-2 | |
| 1.00E-08 | 1 | 4.64148203 | 0.00000007 |
| 7.38E-04 | 0.9993 | 4.58852792 | 0.00001959 |
| 1.48E-03 | 0.9985 | 4.53627500 | 0.00007748 |
| 2.21E-03 | 0.9978 | 4.48471717 | 0.00017278 |
| 2.95E-03 | 0.997 | 4.43384673 | 0.00030453 |
| 3.69E-03 | 0.9963 | 4.38365661 | 0.00047181 |
| 0.3396 | 0.6604 | -0.13905683 | 0.41166015 |
| 0.4717 | 0.5283 | -0.14777537 | 0.41316214 |
| 0.6038 | 0.3962 | -0.08022288 | 0.33168009 |
| 0.7358 | 0.2642 | -0.02319357 | 0.21446242 |
| 0.8679 | 0.1321 | -0.00099661 | 0.12409338 |
| 1 | 1.00E-08 | 0.00000000 | 0.10095576 |
| | | $\alpha$-pinene-OS-3 | |
| 1.00E-08 | 1 | 3.34327061 | 0.00000007 |
| 9.27E-04 | 0.9991 | 3.27330652 | 0.00003256 |
| 1.86E-03 | 0.9981 | 3.20456294 | 0.00012857 |
| 2.78E-03 | 0.9972 | 3.13702604 | 0.00028597 |
| 3.71E-03 | 0.9963 | 3.07068090 | 0.00050267 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln\gamma^{I}$(org) | $\ln\gamma^{I}(H_2O)$ |
|---|---|---|---|
| 4.64E-03 | 0.9954 | 3.00551141 | 0.00077663 |
| 0.2414 | 0.7586 | -0.94679384 | 0.27242378 |
| 0.3931 | 0.6069 | -0.80215482 | 0.19062734 |
| 0.5448 | 0.4552 | -0.43626808 | -0.14198733 |
| 0.6966 | 0.3034 | -0.15397771 | -0.60953333 |
| 0.8483 | 0.1517 | -0.02555762 | -1.05639976 |
| 1 | 1.00E-08 | 0.00000000 | -1.42407901 |
| $\alpha$-pinene-OS-4 | | | |
| 1.00E-08 | 1 | 4.80714672 | 0.00000007 |
| 5.20E-04 | 0.9995 | 4.77592096 | 0.00000817 |
| 1.04E-03 | 0.999 | 4.74487245 | 0.00003236 |
| 1.56E-03 | 0.9984 | 4.71400190 | 0.00007249 |
| 2.08E-03 | 0.9979 | 4.68330940 | 0.00012838 |
| 2.60E-03 | 0.9974 | 4.65279497 | 0.00019987 |
| 0.4378 | 0.5622 | -0.47339566 | 0.57347139 |
| 0.5502 | 0.4498 | -0.40747728 | 0.50420549 |
| 0.6627 | 0.3373 | -0.25659803 | 0.26790042 |
| 0.7751 | 0.2249 | -0.10843509 | -0.10850990 |
| 0.8876 | 0.1124 | -0.02388086 | -0.51026669 |
| 1 | 1.00E-08 | 0.00000000 | -0.85853086 |
| $\alpha$-pinene-OS-5 | | | |
| 1.00E-08 | 1 | 3.40187659 | 0.00000007 |
| 1.35E-03 | 0.9987 | 3.31097218 | 0.00006137 |
| 2.69E-03 | 0.9973 | 3.22203769 | 0.00024188 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^{I}$(org) | $\ln \gamma^{I}(H_2O)$ |
|---|---|---|---|
| 4.03E-03 | 0.996 | 3.13508776 | 0.00053652 |
| 5.38E-03 | 0.9946 | 3.05012830 | 0.00094015 |
| 6.72E-03 | 0.9933 | 2.96715533 | 0.00144768 |
| 0.2268 | 0.7732 | -0.55115713 | 0.25194749 |
| 0.3815 | 0.6185 | -0.55708803 | 0.24183094 |
| 0.5361 | 0.4639 | -0.33473359 | 0.04562307 |
| 0.6907 | 0.3093 | -0.13044047 | -0.28176504 |
| 0.8454 | 0.1546 | -0.02507538 | -0.63145548 |
| 1 | 1.00E-08 | 0.00000000 | -0.93833312 |
| | | $\alpha$-pinene-OS-6 | |
| 1.00E-08 | 1 | 2.76051800 | 0.00000007 |
| 1.39E-03 | 0.9986 | 2.66497968 | 0.00006594 |
| 2.77E-03 | 0.9972 | 2.57175691 | 0.00025950 |
| 4.16E-03 | 0.9958 | 2.48084905 | 0.00057464 |
| 5.54E-03 | 0.9945 | 2.39224474 | 0.00100533 |
| 6.93E-03 | 0.9931 | 2.30592136 | 0.00154561 |
| 0.21 | 0.79 | -1.10577811 | 0.23036603 |
| 0.368 | 0.632 | -1.06449898 | 0.19410079 |
| 0.526 | 0.474 | -0.67829589 | -0.13304361 |
| 0.684 | 0.316 | -0.28410665 | -0.74338900 |
| 0.842 | 0.158 | -0.05869257 | -1.45991421 |
| 1 | 1.00E-08 | 0.00000000 | -2.10954675 |
| | | $\beta$-pinene-OS-1 | |
| 1.00E-08 | 1 | 5.68997377 | 0.00000007 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^{I}$(org) | $\ln \gamma^{I}(H_2O)$ |
|---|---|---|---|
| 3.45E-04 | 0.9997 | 5.65885767 | 0.00000545 |
| 6.90E-04 | 0.9993 | 5.62795753 | 0.00002150 |
| 1.03E-03 | 0.999 | 5.59727351 | 0.00004806 |
| 1.38E-03 | 0.9986 | 5.56680486 | 0.00008500 |
| 1.72E-03 | 0.9983 | 5.53655113 | 0.00013218 |
| 0.3907 | 0.6093 | 0.11356151 | 0.49383968 |
| 0.5126 | 0.4874 | 0.07498509 | 0.52450834 |
| 0.6344 | 0.3656 | 0.06057360 | 0.54605000 |
| 0.7563 | 0.2437 | 0.03750802 | 0.60512119 |
| 0.8781 | 0.1219 | 0.01099184 | 0.73598327 |
| 1 | 1.00E-08 | 0.00000000 | 0.92227144 |
| | | $\beta$-pinene-OS-2 | |
| 1.00E-08 | 1 | 4.45448952 | 0.00000007 |
| 6.11E-04 | 0.9994 | 4.40982444 | 0.00001369 |
| 1.22E-03 | 0.9988 | 4.36564937 | 0.00005415 |
| 1.83E-03 | 0.9982 | 4.32196049 | 0.00012091 |
| 2.44E-03 | 0.9976 | 4.27875342 | 0.00021339 |
| 3.05E-03 | 0.9969 | 4.23602351 | 0.00033106 |
| 0.3593 | 0.6407 | -0.53198665 | 0.44250803 |
| 0.4875 | 0.5125 | -0.50254423 | 0.40884389 |
| 0.6156 | 0.3844 | -0.34573580 | 0.20206244 |
| 0.7437 | 0.2563 | -0.16000620 | -0.20423606 |
| 0.8719 | 0.1281 | -0.03580048 | -0.72346451 |
| 1 | 1.00E-08 | 0.00000000 | -1.19208229 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^I$(org) | $\ln \gamma^I(H_2O)$ |
|---|---|---|---|
| limonene-OS-1 | | | |
| 1.00E-08 | 1 | 5.01896878 | 0.00000007 |
| 5.05E-04 | 0.9995 | 4.97944907 | 0.00001003 |
| 1.01E-03 | 0.999 | 4.94029114 | 0.00003968 |
| 1.51E-03 | 0.9985 | 4.90149379 | 0.00008867 |
| 2.02E-03 | 0.998 | 4.86305504 | 0.00015667 |
| 2.52E-03 | 0.9975 | 4.82497263 | 0.00024334 |
| 0.3724 | 0.6276 | -0.16974861 | 0.46362004 |
| 0.4979 | 0.5021 | -0.16297273 | 0.45411651 |
| 0.6235 | 0.3765 | -0.09319285 | 0.36123235 |
| 0.749 | 0.251 | -0.03195072 | 0.22383694 |
| 0.8745 | 0.1255 | -0.00442394 | 0.10235441 |
| 1 | 1.00E-08 | 0.00000000 | 0.04181320 |
| limonene-OS-2 | | | |
| 1.00E-08 | 1 | 5.21158102 | 0.00000007 |
| 3.83E-04 | 0.9996 | 5.17811329 | 0.00000649 |
| 7.67E-04 | 0.9992 | 5.14489369 | 0.00002564 |
| 1.15E-03 | 0.9988 | 5.11192213 | 0.00005734 |
| 1.53E-03 | 0.9985 | 5.07919780 | 0.00010139 |
| 1.92E-03 | 0.9981 | 5.04671962 | 0.00015763 |
| 0.3625 | 0.6375 | -0.19574436 | 0.44849806 |
| 0.49 | 0.51 | -0.16781332 | 0.42309796 |
| 0.6175 | 0.3825 | -0.08152360 | 0.31101061 |
| 0.745 | 0.255 | -0.01489144 | 0.15945573 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^{I}$(org) | $\ln \gamma^{I}(H_2O)$ |
|---|---|---|---|
| 0.8725 | 0.1275 | 0.00704862 | 0.04119941 |
| 1 | 1.00E-08 | 0.00000000 | 0.00826903 |
| | | limonene-OS-3 | |
| 1.00E-08 | 1 | 5.87725874 | 0.00000007 |
| 2.32E-04 | 0.9998 | 5.85372965 | 0.00000280 |
| 4.64E-04 | 0.9995 | 5.83031494 | 0.00001095 |
| 6.96E-04 | 0.9993 | 5.80701536 | 0.00002448 |
| 9.28E-04 | 0.9991 | 5.78383069 | 0.00004332 |
| 1.16E-03 | 0.9988 | 5.76076064 | 0.00006743 |
| 0.3763 | 0.6237 | -0.02139778 | 0.47099664 |
| 0.501 | 0.499 | -0.01382572 | 0.46249432 |
| 0.6258 | 0.3742 | 0.01401673 | 0.42797760 |
| 0.7505 | 0.2495 | 0.01792621 | 0.42671848 |
| 0.8753 | 0.1247 | 0.00512185 | 0.50137643 |
| 1 | 1.00E-08 | 0.00000000 | 0.63305556 |
| | | limonene-OS-4 | |
| 1.00E-08 | 1 | 5.35708475 | 0.00000007 |
| 2.96E-04 | 0.9997 | 5.33038275 | 0.00000402 |
| 5.92E-04 | 0.9994 | 5.30383423 | 0.00001581 |
| 8.88E-04 | 0.9991 | 5.27743972 | 0.00003535 |
| 1.18E-03 | 0.9988 | 5.25119877 | 0.00006255 |
| 1.48E-03 | 0.9985 | 5.22511068 | 0.00009732 |
| 0.3843 | 0.6157 | -0.33421220 | 0.48362181 |
| 0.5074 | 0.4926 | -0.28938819 | 0.43804153 |

**Table S3 – continued from previous page**

| $x$(org) | $x$($H_2O$) | $\ln\gamma^I$(org) | $\ln\gamma^I$($H_2O$) |
|---|---|---|---|
| 0.6306 | 0.3694 | -0.17284521 | 0.27478729 |
| 0.7537 | 0.2463 | -0.06656310 | 0.02867420 |
| 0.8769 | 0.1231 | -0.01158726 | -0.21779401 |
| 1 | 1.00E-08 | 0.00000000 | -0.40900861 |
| | | isoprene-OS-1 | |
| 1.00E-08 | 1 | 1.38344406 | 0.00000007 |
| 0.05 | 0.95 | 0.32144684 | 0.02394751 |
| 0.15 | 0.85 | -0.44833226 | 0.09927954 |
| 0.25 | 0.75 | -0.61110043 | 0.13526486 |
| 0.35 | 0.65 | -0.56239206 | 0.11117103 |
| 0.45 | 0.55 | -0.43229078 | 0.02205117 |
| 0.55 | 0.45 | -0.28567331 | -0.12605092 |
| 0.65 | 0.35 | -0.16027294 | -0.31448215 |
| 0.75 | 0.25 | -0.07273609 | -0.51771424 |
| 0.85 | 0.15 | -0.02285551 | -0.71472290 |
| 0.95 | 0.05 | -0.00226949 | -0.89444067 |
| 1 | 1.00E-08 | 0.00000000 | -0.97653593 |
| | | isoprene-OS-2 | |
| 1.00E-08 | 1 | 0.89819266 | 0.00000007 |
| 0.05 | 0.95 | -0.22386930 | 0.02508034 |
| 0.15 | 0.85 | -0.95177361 | 0.09612947 |
| 0.25 | 0.75 | -1.02070596 | 0.10994303 |
| 0.35 | 0.65 | -0.85545260 | 0.03694763 |
| 0.45 | 0.55 | -0.60645970 | -0.13095701 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^I$(org) | $\ln \gamma^I(H_2O)$ |
|---|---|---|---|
| 0.55 | 0.45 | -0.36614515 | -0.37269105 |
| 0.65 | 0.35 | -0.18764655 | -0.64098077 |
| 0.75 | 0.25 | -0.07908318 | -0.89396116 |
| 0.85 | 0.15 | -0.02366416 | -1.11422459 |
| 0.95 | 0.05 | -0.00230280 | -1.30150283 |
| 1 | 1.00E-08 | 0.00000000 | -1.38373509 |
| | isoprene-OS-3 | | |
| 1.00E-08 | 1 | -0.41196228 | 0.00000007 |
| 0.05 | 0.95 | -0.97865783 | 0.01121896 |
| 0.15 | 0.85 | -1.05947270 | 0.01414716 |
| 0.25 | 0.75 | -0.81769233 | -0.04704571 |
| 0.35 | 0.65 | -0.54745110 | -0.16424797 |
| 0.45 | 0.55 | -0.32434986 | -0.31680182 |
| 0.55 | 0.45 | -0.16680632 | -0.48174616 |
| 0.65 | 0.35 | -0.06870731 | -0.64167124 |
| 0.75 | 0.25 | -0.01569136 | -0.78758648 |
| 0.85 | 0.15 | 0.00589515 | -0.91700462 |
| 0.95 | 0.05 | 0.00598847 | -1.03085868 |
| 1 | 1.00E-08 | 0.00000000 | -1.08259251 |
| | isoprene-OS-4 | | |
| 1.00E-08 | 1 | 0.21417729 | 0.00000007 |
| 0.05 | 0.95 | -0.32793875 | 0.01206830 |
| 0.15 | 0.85 | -0.63285155 | 0.03998876 |
| 0.25 | 0.75 | -0.59936913 | 0.02921238 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^{I}$(org) | $\ln \gamma^{I}(H_2O)$ |
|---|---|---|---|
| 0.35 | 0.65 | -0.47173317 | -0.02627195 |
| 0.45 | 0.55 | -0.33023171 | -0.11994821 |
| 0.55 | 0.45 | -0.20752311 | -0.24043961 |
| 0.65 | 0.35 | -0.11512777 | -0.37509995 |
| 0.75 | 0.25 | -0.05345091 | -0.51310769 |
| 0.85 | 0.15 | -0.01778959 | -0.64712191 |
| 0.95 | 0.05 | -0.00210553 | -0.77323149 |
| 1 | 1.00E-08 | 0.00000000 | -0.83280603 |
| cis-$\beta$-IEPOX | | | |
| 1.00E-08 | 1 | -0.06607103 | 0.00000007 |
| 0.05 | 0.95 | -0.00540659 | -0.00150073 |
| 0.15 | 0.85 | 0.02351606 | -0.00346604 |
| 0.25 | 0.75 | -0.01141428 | 0.00507173 |
| 0.35 | 0.65 | -0.03779131 | 0.01526326 |
| 0.45 | 0.55 | -0.04434317 | 0.01808982 |
| 0.55 | 0.45 | -0.03768554 | 0.00965761 |
| 0.65 | 0.35 | -0.02563953 | -0.01036402 |
| 0.75 | 0.25 | -0.01366817 | -0.04050680 |
| 0.85 | 0.15 | -0.00481492 | -0.07864690 |
| 0.95 | 0.05 | -0.00041435 | -0.12262604 |
| 1 | 1.00E-08 | 0.00000000 | -0.14619588 |
| trans-$\beta$-IEPOX | | | |
| 1.00E-08 | 1 | -0.11502697 | 0.00000007 |
| 0.05 | 0.95 | -0.03167926 | -0.00211193 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^I$(org) | $\ln \gamma^I(H_2O)$ |
|---|---|---|---|
| 0.15 | 0.85 | 0.01975114 | -0.00674026 |
| 0.25 | 0.75 | -0.01039226 | 0.00028072 |
| 0.35 | 0.65 | -0.03770694 | 0.01073065 |
| 0.45 | 0.55 | -0.04590063 | 0.01489269 |
| 0.55 | 0.45 | -0.04017262 | 0.00816962 |
| 0.65 | 0.35 | -0.02827853 | -0.01013829 |
| 0.75 | 0.25 | -0.01591409 | -0.03864826 |
| 0.85 | 0.15 | -0.00632601 | -0.07518676 |
| 0.95 | 0.05 | -0.00096277 | -0.11751679 |
| 1 | 1.00E-08 | 0.00000000 | -0.14022541 |
| | | $\delta_1$-IEPOX | |
| 1.00E-08 | 1 | -0.96786087 | 0.00000006 |
| 0.05 | 0.95 | -0.70766384 | -0.00614888 |
| 0.15 | 0.85 | -0.41478481 | -0.03495589 |
| 0.25 | 0.75 | -0.28853434 | -0.06422185 |
| 0.35 | 0.65 | -0.21401489 | -0.09443639 |
| 0.45 | 0.55 | -0.15579014 | -0.13056960 |
| 0.55 | 0.45 | -0.10680053 | -0.17457643 |
| 0.65 | 0.35 | -0.06689998 | -0.22587768 |
| 0.75 | 0.25 | -0.03657942 | -0.28272363 |
| 0.85 | 0.15 | -0.01564090 | -0.34320634 |
| 0.95 | 0.05 | -0.00328635 | -0.40576005 |
| 1 | 1.00E-08 | 0.00000000 | -0.43746403 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^{I}$(org) | $\ln \gamma^{I}(H_2O)$ |
|---|---|---|---|
| | $\delta_4$-IEPOX | | |
| 1.00E-08 | 1 | -0.18735760 | 0.00000006 |
| 0.05 | 0.95 | -0.05275575 | -0.00291807 |
| 0.15 | 0.85 | 0.02779607 | -0.00908656 |
| 0.25 | 0.75 | 0.00977799 | -0.00428701 |
| 0.35 | 0.65 | -0.01241106 | 0.00371545 |
| 0.45 | 0.55 | -0.02154561 | 0.00732844 |
| 0.55 | 0.45 | -0.02048365 | 0.00327313 |
| 0.65 | 0.35 | -0.01453802 | -0.00900165 |
| 0.75 | 0.25 | -0.00773642 | -0.02870865 |
| 0.85 | 0.15 | -0.00250120 | -0.05453296 |
| 0.95 | 0.05 | -0.00003856 | -0.08505944 |
| 1 | 1.00E-08 | 0.00000000 | -0.10167232 |
| | Methyl bisulfate | | |
| 1.00E-08 | 1 | 0.55835039 | 0.00000002 |
| 0.05 | 0.95 | -0.14847044 | 0.01668245 |
| 0.15 | 0.85 | -0.85943025 | 0.09005165 |
| 0.25 | 0.75 | -1.14690289 | 0.15882766 |
| 0.35 | 0.65 | -1.22465306 | 0.18952024 |
| 0.45 | 0.55 | -1.15490370 | 0.13929634 |
| 0.55 | 0.45 | -0.92841316 | -0.09502714 |
| 0.65 | 0.35 | -0.54918590 | -0.67366264 |
| 0.75 | 0.25 | -0.22800395 | -1.41999653 |
| 0.85 | 0.15 | -0.06108956 | -2.07584590 |

**Table S3 – continued from previous page**

| $x$(org) | $x(H_2O)$ | $\ln \gamma^I$(org) | $\ln \gamma^I(H_2O)$ |
|---|---|---|---|
| 0.95 | 0.05 | -0.00447075 | -2.56437274 |
| 1 | 1.00E-08 | 0.00000000 | -2.71866247 |

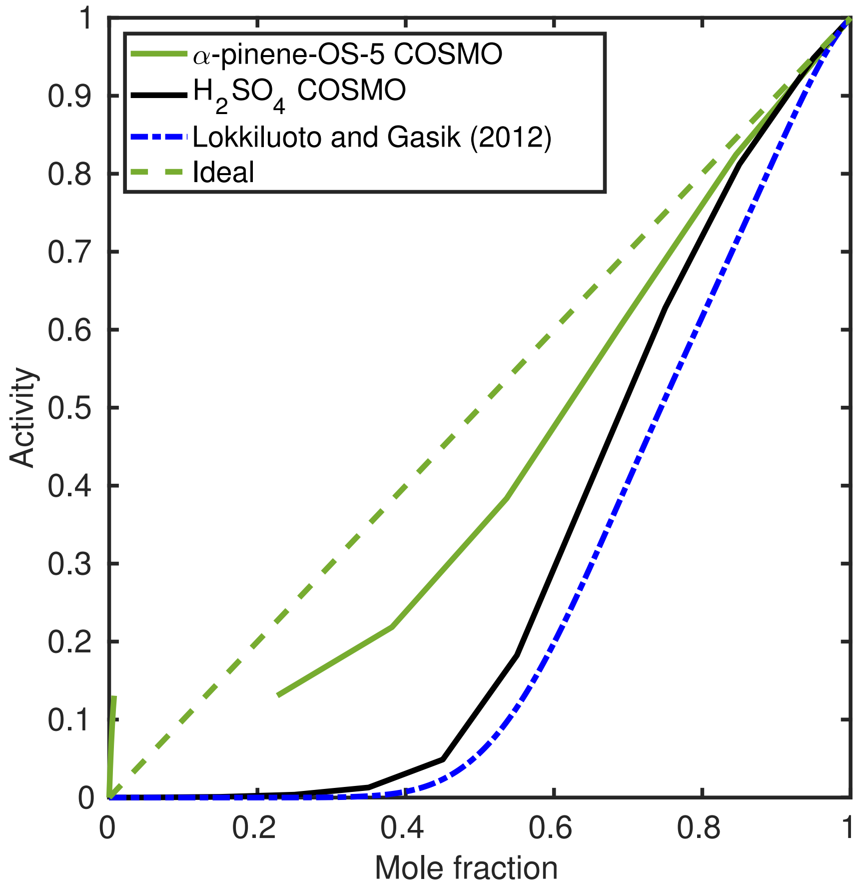


Figure S6: Comparison between COSMO*therm* calculated $\alpha$-pinene-OS-5 and $H_2SO_4$ activities, and literature values[S4] of $H_2SO_4$ activities in pure water ($T$ = 298.15 K). Note that the experimentally derived activity coefficients include the effects from the dissociation of sulfuric acid.

**Table S4: Activity coefficients of the organics and water in ternary aqueous 0.09 mole fraction ammonium bisulfate solutions, at 298.15 K. Note that the mole fractions and activity coefficients are given in the COSMO*therm* framework, and should be converted using Equations S7 and S8, respectively. However, the activities can be calculated using either (Equation S6).**

| $x$'(org) | $x$'($H_2O$) | $\ln\gamma^{I}$'(org) | $\ln\gamma^{I}$'($H_2O$) |
|---|---|---|---|
| | | $\alpha$-pinene-OS-5 | |
| 0 | 0.8349 | 6.93440625 | -0.07148410 |
| 9.76E-05 | 0.8348 | 6.92670895 | -0.07172677 |
| 1.95E-04 | 0.8347 | 6.91901613 | -0.07196911 |
| 2.93E-04 | 0.8346 | 6.91132789 | -0.07221112 |
| 3.90E-04 | 0.8345 | 6.90364431 | -0.07245278 |
| 4.88E-04 | 0.8345 | 6.89596540 | -0.07269410 |
| 0.5244 | 0.3971 | -0.08374992 | -0.24283688 |
| 0.6195 | 0.3177 | -0.05750087 | -0.38050631 |
| 0.7146 | 0.2382 | -0.02888838 | -0.53204176 |
| 0.8098 | 0.1588 | -0.00986429 | -0.68085238 |
| 0.9049 | 0.0794 | -0.00119644 | -0.81753428 |
| 1 | 0 | 0.00000000 | -0.93833314 |
| | | $\beta$-pinene-OS-1 | |
| 0 | 0.8349 | 9.34043829 | -0.07148410 |
| 1.61E-05 | 0.8348 | 9.33892278 | -0.07152657 |
| 3.22E-05 | 0.8348 | 9.33740746 | -0.07156904 |
| 4.83E-05 | 0.8348 | 9.33589233 | -0.07161149 |
| 6.44E-05 | 0.8348 | 9.33437740 | -0.07165392 |
| 8.04E-05 | 0.8348 | 9.33286265 | -0.07169634 |
| 0.8813 | 0.0991 | 0.03128335 | 0.58519254 |

**Table S4 – continued from previous page**

| $x$'(org) | $x$'($H_2O$) | $\ln \gamma^{I}$'(org) | $\ln \gamma^{I}$'($H_2O$) |
|---|---|---|---|
| 0.905 | 0.0793 | 0.02044998 | 0.64331224 |
| 0.9288 | 0.0595 | 0.01168913 | 0.70638528 |
| 0.9525 | 0.0397 | 0.00522123 | 0.77420323 |
| 0.9763 | 0.0198 | 0.00126136 | 0.84636938 |
| 1 | 0 | 0.00000000 | 0.92227145 |

limonene-OS-1

| | | | |
|---|---|---|---|
| 0 | 0.8349 | 8.56540801 | -0.07148410 |
| 2.93E-05 | 0.8348 | 8.56303445 | -0.07155621 |
| 5.86E-05 | 0.8348 | 8.56066103 | -0.07162828 |
| 8.79E-05 | 0.8348 | 8.55828778 | -0.07170033 |
| 1.17E-04 | 0.8348 | 8.55591474 | -0.07177234 |
| 1.47E-04 | 0.8347 | 8.55354187 | -0.07184432 |
| 0.7249 | 0.2297 | 0.04705734 | 0.01370163 |
| 0.7799 | 0.1838 | 0.03378174 | -0.00986050 |
| 0.8349 | 0.1378 | 0.02178422 | -0.02382205 |
| 0.8899 | 0.0919 | 0.01112840 | -0.02276621 |
| 0.945 | 0.0459 | 0.00310955 | -0.00184360 |
| 1 | 0 | 0.00000000 | 0.04181320 |

isoprene-OS-2

| | | | |
|---|---|---|---|
| 0 | 0.8349 | 3.82228285 | -0.07148410 |
| 1.76E-03 | 0.8334 | 3.74309497 | -0.07556788 |
| 3.53E-03 | 0.8319 | 3.66551171 | -0.07953377 |
| 5.29E-03 | 0.8304 | 3.58950234 | -0.08338449 |
| 7.06E-03 | 0.829 | 3.51504096 | -0.08712259 |

**Table S4 – continued from previous page**

| $x$'(org) | $x$'($H_2O$) | $\ln \gamma^{I}$'(org) | $\ln \gamma^{I}$'($H_2O$) |
|---|---|---|---|
| 8.82E-03 | 0.8275 | 3.44209791 | -0.09075080 |
| 0.3249 | 0.5636 | -0.16419350 | -0.31849729 |
| 0.4599 | 0.4509 | -0.15632112 | -0.52596279 |
| 0.5949 | 0.3382 | -0.06944642 | -0.79729730 |
| 0.73 | 0.2254 | -0.01597782 | -1.05299975 |
| 0.865 | 0.1127 | -0.00093741 | -1.24860285 |
| 1 | 0 | 0.00000000 | -1.38373510 |
| | | $\delta_1$-IEPOX | |
| 0 | 0.8349 | 0.84847604 | -0.07148410 |
| 0.05 | 0.7931 | 0.67644880 | -0.13567635 |
| 0.15 | 0.7096 | 0.40802408 | -0.22637132 |
| 0.25 | 0.6261 | 0.27811744 | -0.28766514 |
| 0.35 | 0.5427 | 0.19334052 | -0.33627708 |
| 0.45 | 0.4592 | 0.13230859 | -0.37708178 |
| 0.55 | 0.3757 | 0.08579571 | -0.41142791 |
| 0.65 | 0.2922 | 0.04971065 | -0.43872772 |
| 0.75 | 0.2087 | 0.02273707 | -0.45706549 |
| 0.85 | 0.1252 | 0.00512517 | -0.46326792 |
| 0.95 | 0.0417 | -0.00155910 | -0.45214155 |
| 1 | 0 | 0.00000000 | -0.43746404 |

**Table S5: Activity coefficients of the organics and water in ternary aqueous 0.09 mole fraction ammonium sulfate solutions, at 298.15 K. Note that the mole fractions and activity coefficients are given in the COSMO*therm* framework, and should be converted using Equations S7 and S8, respectively. However, the activities can be calculated using either (Equation S6).**

| $x$'(org) | $x$'($H_2O$) | ln $\gamma^{I}$'(org) | ln $\gamma^{I}$'($H_2O$) |
|---|---|---|---|
| | $\alpha$-pinene-OS-5 | | |
| 0 | 0.7712 | 10.9746567 | 0.38650676 |
| 2.64E-06 | 0.7712 | 10.97425201 | 0.38648605 |
| 5.27E-06 | 0.7712 | 10.97384651 | 0.38646537 |
| 7.91E-06 | 0.7712 | 10.97344102 | 0.38644469 |
| 1.05E-05 | 0.7712 | 10.97303554 | 0.38642402 |
| 1.32E-05 | 0.7712 | 10.972627 | 0.38640318 |
| 0.6573 | 0.2643 | 0.15503718 | -0.55855118 |
| 0.726 | 0.2113 | 0.11603024 | -0.69706966 |
| 0.7945 | 0.1585 | 0.07475409 | -0.81081242 |
| 0.863 | 0.1057 | 0.04004649 | -0.89719833 |
| 0.9315 | 0.0528 | 0.01477921 | -0.95353053 |
| 1 | 0 | 0 | -0.93833314 |
| | $\beta$-pinene-OS-1 | | |
| 0 | 0.7712 | 13.62597811 | 0.38650676 |
| 2.38E-07 | 0.7712 | 13.62593646 | 0.3865048 |
| 4.76E-07 | 0.7712 | 13.62589411 | 0.38650287 |
| 7.14E-07 | 0.7712 | 13.62585176 | 0.38650093 |
| 9.52E-07 | 0.7712 | 13.6258094 | 0.386499 |
| 1.19E-06 | 0.7712 | 13.62576705 | 0.38649707 |
| 0.9809 | 0.0147 | 0.00350281 | 0.78810383 |

**Table S5 – continued from previous page**

| $x$'(org) | $x$'($H_2O$) | $\ln \gamma^{I}$'(org) | $\ln \gamma^{I}$'($H_2O$) |
|---|---|---|---|
| 0.9847 | 0.0118 | 0.00244294 | 0.80859989 |
| 0.9885 | 8.83E-03 | 0.00152435 | 0.83110332 |
| 0.9924 | 5.89E-03 | 0.0007718 | 0.85632922 |
| 0.9962 | 2.94E-03 | 0.00022908 | 0.88562421 |
| 1 | 0 | 0 | 0.92227145 |
| | | limonene-OS-1 | |
| 0 | 0.7712 | 13.21198231 | 0.38650676 |
| 3.46E-07 | 0.7712 | 13.21192412 | 0.38650385 |
| 6.92E-07 | 0.7712 | 13.2118652 | 0.38650097 |
| 1.04E-06 | 0.7712 | 13.21180627 | 0.38649809 |
| 1.38E-06 | 0.7712 | 13.21174735 | 0.3864952 |
| 1.73E-06 | 0.7712 | 13.21168843 | 0.38649232 |
| 0.9241 | 0.0585 | 0.02346932 | -0.12346386 |
| 0.9393 | 0.0468 | 0.01707799 | -0.11453178 |
| 0.9545 | 0.0351 | 0.0113298 | -0.09987282 |
| 0.9697 | 0.0234 | 0.00631327 | -0.07669965 |
| 0.9848 | 0.0117 | 0.00224958 | -0.03853834 |
| 1 | 0 | 0 | 0.0418132 |
| | | isoprene-OS-2 | |
| 0 | 0.7712 | 6.36107283 | 0.38650676 |
| 1.76E-04 | 0.7711 | 6.34687248 | 0.38549488 |
| 3.52E-04 | 0.7709 | 6.33269604 | 0.38448634 |
| 5.28E-04 | 0.7708 | 6.31854383 | 0.3834811 |
| 7.04E-04 | 0.7706 | 6.30441632 | 0.38247916 |

**Table S5 – continued from previous page**

| $x$'(org) | $x$'($H_2O$) | $\ln \gamma^{I}$'(org) | $\ln \gamma^{I}$'($H_2O$) |
|---|---|---|---|
| 8.81E-04 | 0.7705 | 6.29027928 | 0.38147808 |
| 0.4399 | 0.432 | 0.07719509 | -0.38817693 |
| 0.5517 | 0.3457 | 0.12851291 | -0.70458111 |
| 0.6638 | 0.2593 | 0.13528186 | -1.0211394 |
| 0.7759 | 0.1729 | 0.08662511 | -1.26899869 |
| 0.8879 | 0.0864 | 0.03237511 | -1.41924685 |
| 1 | 0 | 0 | -1.3837351 |
| | $\delta_1$-IEPOX | | |
| 0 | 0.7712 | 4.57475479 | 0.38650676 |
| 2.68E-03 | 0.7691 | 4.50581095 | 0.37113771 |
| 5.35E-03 | 0.7671 | 4.43876863 | 0.35612251 |
| 8.03E-03 | 0.765 | 4.37353962 | 0.34144688 |
| 0.0107 | 0.7629 | 4.31003384 | 0.3270975 |
| 0.0134 | 0.7609 | 4.24765149 | 0.31294408 |
| 0.8874 | 0.0868 | 0.05339775 | -0.64201559 |
| 0.91 | 0.0694 | 0.0386952 | -0.63139267 |
| 0.9325 | 0.0521 | 0.02550655 | -0.61443628 |
| 0.955 | 0.0347 | 0.01401898 | -0.58730439 |
| 0.9775 | 0.0174 | 0.0047697 | -0.54088997 |
| 1 | 0 | 0 | -0.43746404 |

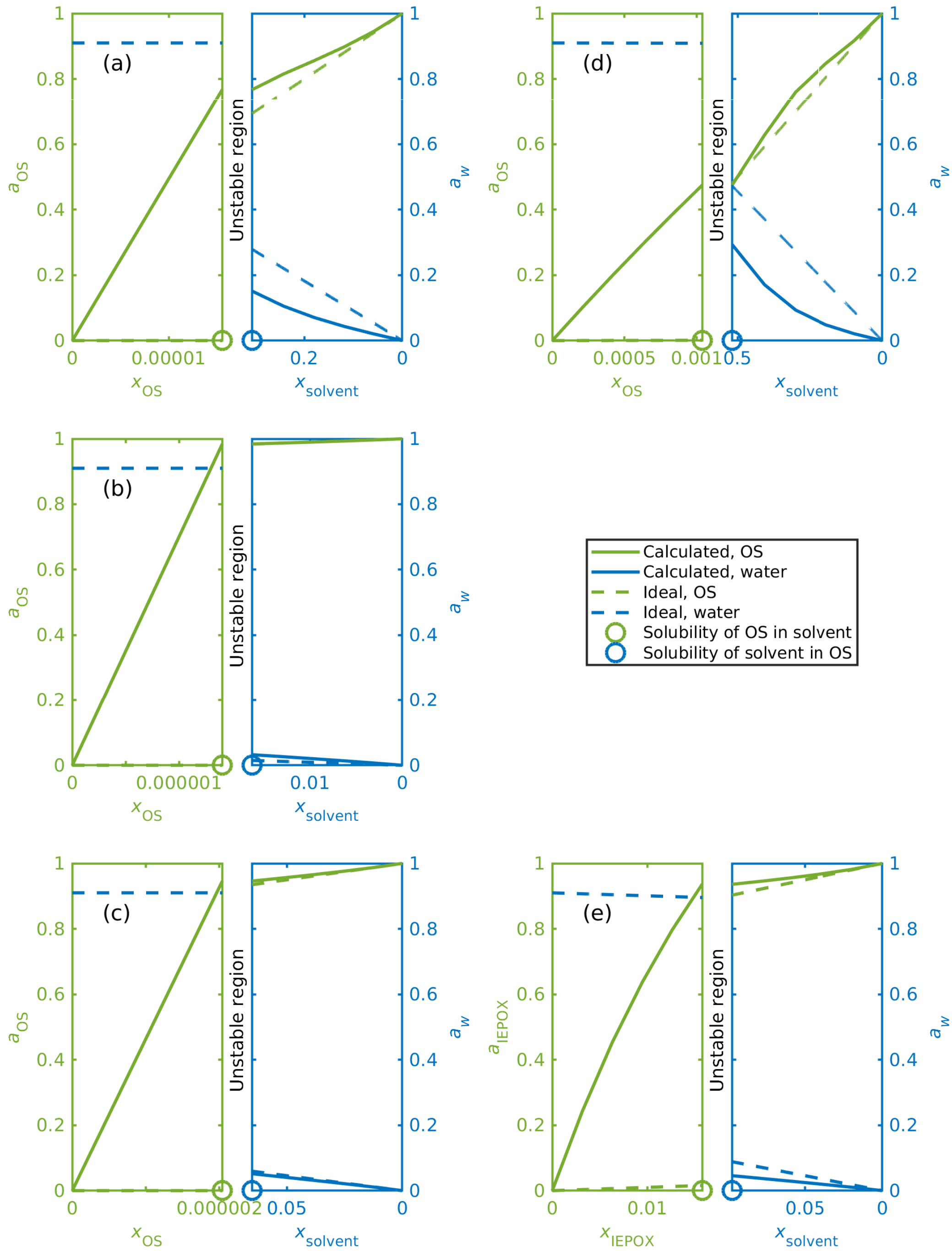


Figure S7: The activities of the OS and IEPOX, and water in ternary mixtures. The solvent is a 0.09 mole fraction ammonium sulfate and the ideal water activity is equal to the mole fraction of water. a) $\alpha$-pinene-OS-5, b) $\beta$-pinene-OS-1, c) limonene-OS-1, d) isoprene-OS-2, e) $\delta_1$-IEPOX. The left panel of each figure shows the solvent-rich phase and the right panel the organic-rich phase.The predicted activity of water in the solvent-rich phase is 1.14, which is outside the scale of the figures.

**Table S6: Activity coefficients of the organic compounds in the infinite dilution of water, free energies of solvation and Henry's law solubilities calculated with different methods. The free energies are given in units of kcal/mol and the Henry's law solubilities in mol/m$^3$Pa.**

| | $\gamma^{\mathrm{I}}(0)$ | $G_{\mathrm{solv}}$ | $H_{\mathrm{sol}}^{\infty}$ | $H_{\mathrm{sol}}^{LLE}$ |
|---|---|---|---|---|
| $\alpha$-pinene-OS-1 | 516.64 | -14.36 | $1.35 \cdot 10^{7}$ | $6.46 \cdot 10^{6}$ |
| $\alpha$-pinene-OS-2 | 103.70 | -14.76 | $2.66 \cdot 10^{7}$ | $8.98 \cdot 10^{6}$ |
| $\alpha$-pinene-OS-3 | 28.31 | -19.99 | $1.81 \cdot 10^{11}$ | $2.08 \cdot 10^{10}$ |
| $\alpha$-pinene-OS-4 | 122.38 | -18.30 | $1.05 \cdot 10^{10}$ | $2.96 \cdot 10^{9}$ |
| $\alpha$-pinene-OS-5 | 30.02 | -20.39 | $3.55 \cdot 10^{11}$ | $6.13 \cdot 10^{10}$ |
| $\alpha$-pinene-OS-6 | 15.81 | -21.56 | $2.56 \cdot 10^{12}$ | $2.39 \cdot 10^{11}$ |
| $\beta$-pinene-OS-1 | 295.89 | -15.15 | $5.12 \cdot 10^{7}$ | $2.34 \cdot 10^{7}$ |
| $\beta$-pinene-OS-2 | 86.01 | -15.14 | $5.01 \cdot 10^{7}$ | $1.17 \cdot 10^{7}$ |
| limonene-OS-1 | 151.26 | -15.38 | $7.55 \cdot 10^{7}$ | $2.57 \cdot 10^{7}$ |
| limonene-OS-2 | 183.38 | -15.82 | $1.60 \cdot 10^{8}$ | $5.04 \cdot 10^{7}$ |
| limonene-OS-3 | 356.83 | -15.62 | $1.14 \cdot 10^{8}$ | $4.24 \cdot 10^{7}$ |
| limonene-OS-4 | 212.11 | -15.44 | $8.40 \cdot 10^{7}$ | $2.37 \cdot 10^{7}$ |
| isoprene-OS-1 | 3.99 | -18.16 | $8.26 \cdot 10^{9}$ | - |
| isoprene-OS-2 | 2.46 | -16.94 | $1.05 \cdot 10^{9}$ | - |
| isoprene-OS-3 | 0.66 | -21.73 | $3.45 \cdot 10^{12}$ | - |
| isoprene-OS-4 | 1.24 | -21.46 | $2.16 \cdot 10^{12}$ | - |
| Cis-$\beta$-IEPOX | 0.89 | -11.72 | $1.59 \cdot 10^{5}$ | - |
| Trans-$\beta$-IEPOX | 0.94 | -12.00 | $2.52 \cdot 10^{5}$ | - |
| $\delta_1$-IEPOX | 0.38 | -9.80 | $6.20 \cdot 10^{3}$ | - |
| $\delta_4$-IEPOX | 0.83 | -11.70 | $1.51 \cdot 10^{5}$ | - |
| Methyl bisulfate | 1.75 | -10.75 | $3.04 \cdot 10^{4}$ | - |
| Sulfuric acid | $1.56 \cdot 10^{-3}$ | -16.49 | $4.91 \cdot 10^{8}$ | - |

**Table S7: Molar weights ($MW$), and estimated densities ($\rho$) and volumes ($\widetilde{V}$) of the liquid phase compounds at 298.15 K. The experimentally determined density of pure sulfuric acid at 298.15 K is 1.8255.[S5]**

| | $MW$(g/mol) | $\rho$(g/ml) | $\widetilde{V}$(Å$^3$) |
|---|---|---|---|
| $\alpha$-pinene-OS-1 | 250.314 | 1.286 | 321.100 |
| $\alpha$-pinene-OS-2 | 250.314 | 1.284 | 322.023 |
| $\alpha$-pinene-OS-3 | 266.313 | 1.257 | 351.258 |
| $\alpha$-pinene-OS-4 | 280.296 | 1.251 | 363.253 |
| $\alpha$-pinene-OS-5 | 280.296 | 1.317 | 350.871 |
| $\alpha$-pinene-OS-6 | 280.296 | 1.313 | 353.888 |
| $\beta$-pinene-OS-1 | 250.314 | 1.298 | 320.682 |
| $\beta$-pinene-OS-2 | 250.314 | 1.299 | 318.565 |
| limonene-OS-1 | 250.314 | 1.255 | 329.109 |
| limonene-OS-2 | 250.314 | 1.249 | 331.035 |
| limonene-OS-3 | 250.314 | 1.260 | 329.988 |
| limonene-OS-4 | 250.314 | 1.254 | 329.435 |
| isoprene-OS-1 | 198.195 | 1.391 | 234.832 |
| isoprene-OS-2 | 198.195 | 1.385 | 237.445 |
| isoprene-OS-3 | 216.211 | 1.427 | 249.176 |
| isoprene-OS-4 | 216.211 | 1.446 | 244.129 |
| Cis-$\beta$-IEPOX | 118.132 | 1.172 | 167.508 |
| Trans-$\beta$-IEPOX | 118.132 | 1.173 | 167.626 |
| $\delta_1$-IEPOX | 118.132 | 1.142 | 171.970 |
| $\delta_4$-IEPOX | 118.132 | 1.163 | 171.575 |
| Methyl bisulfate | 112.106 | 1.522 | 122.339 |
| Sulfuric acid | 98.079 | 1.958 | 83.180 |

# References


(S1) Toure, O.; Audonnet, F.; Lebert, A.; Dussap, C.-G. COSMO-RS-PDHS: a new predictive model for aqueous electrolytes solutions. *Chem. Eng. Res. Des.* **2014**, *92*, 2873–2883.

(S2) Toure, O.; Audonnet, F.; Lebert, A.; Dussap, C.-G. Development of a thermodynamic model of aqueous solution suited for foods and biological media. Part A: Prediction of activity coefficients in aqueous mixtures containing electrolytes. *Can. J. Chem. Eng.* **2015**, *93*, 443–450.

(S3) Toure, O.; Lebert, A.; Dussap, C.-G. Extension of the COSMO-RS-PDHS model to the prediction of activity coefficients in concentrated {water-electrolyte} and {water-polyol} solutions. *Fluid Phase Equilib.* **2016**, *424*, 90–104.

(S4) Lokkiluoto, A. K. K.; Gasik, M. M. Activities and free energy of mixing of sulfuric acid solutions by Gibbs–Duhem equation integration. *J. Chem. Eng. Data* **2012**, *57*, 1665–1671.

(S5) Perry, R. H.; Green, D. W.; Maloney, J. O. *Perry's Chemical Engineers' Handbook*, 7th ed.; McGraw-Hill New York, 1997.