

Supplementary Information

“Physical Properties of Short Chain Aqueous Organosulfate Aerosol”

Environmental Science: Atmospheres

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Table S1: Measured water activity ($\pm 0.008 a_w$ units) for sodium methyl and ethyl sulfates at various solute mass fractions and calculated growth factors.

| Sodium methyl sulfate | | | Sodium ethyl sulfate | | |
|-----------------------|----------------|-----------------------------|----------------------|----------------|-----------------------------|
| Solute mass fraction | Water activity | Growth factor (D_p/D_0) | Solute mass fraction | Water activity | Growth factor (D_p/D_0) |
| 0 | 0.993 | | 0 | 0.993 | |
| 0.060 | 0.992 | 3.15 | 0.014 | 0.992 | 4.87 |
| 0.090 | 0.992 | 2.73 | 0.080 | 0.992 | 2.70 |
| 0.10 | 0.972 | 2.63 | 0.14 | 0.992 | 2.22 |
| 0.13 | 0.955 | 2.40 | 0.17 | 0.992 | 2.07 |
| 0.14 | 0.983 | 2.33 | 0.20 | 0.985 | 1.95 |
| 0.17 | 0.940 | 2.17 | 0.23 | 0.979 | 1.85 |
| 0.17 | 0.933 | 2.17 | 0.25 | 0.965 | 1.80 |
| 0.20 | 0.914 | 2.07 | 0.28 | 0.958 | 1.72 |
| 0.22 | 0.927 | 1.97 | 0.31 | 0.937 | 1.66 |
| 0.25 | 0.951 | 1.88 | 0.34 | 0.923 | 1.60 |
| 0.27 | 0.909 | 1.82 | 0.39 | 0.880 | 1.51 |
| 0.29 | 0.899 | 1.77 | 0.41 | 0.861 | 1.48 |
| 0.36 | 0.842 | 1.63 | 0.44 | 0.842 | 1.44 |
| 0.38 | 0.831 | 1.59 | 0.48 | 0.816 | 1.39 |
| | | | 0.50 | 0.801 | 1.37 |
| | | | 0.52 | 0.763 | 1.35 |
| | | | 0.55 | 0.720 | 1.31 |

Table S2: Physical parameters for sodium methyl sulfate measured with bulk techniques. *Error on density measurements is 0.0005 g/cm³ **Error on n(589nm) measurements is 0.00005 RI units.

| Solute Mass Fraction | Molar Concentration (M) | Density* (g/cm ³) | n(589nm)** |
|----------------------|-------------------------|-------------------------------|------------|
| 0.00 | 0.00 | 0.998 | 1.3330 |
| 0.02 | 0.15 | 1.011 | 1.3349 |
| 0.03 | 0.23 | 1.017 | 1.3358 |
| 0.04 | 0.30 | 1.023 | 1.3366 |
| 0.06 | 0.45 | 1.035 | 1.3385 |
| 0.08 | 0.61 | 1.047 | 1.3402 |
| 0.10 | 0.79 | 1.060 | 1.3422 |
| 0.17 | 1.40 | 1.107 | 1.3490 |
| 0.20 | 1.68 | 1.129 | 1.3521 |
| 0.25 | 2.17 | 1.164 | 1.3567 |
| 0.29 | 2.58 | 1.192 | 1.3605 |
| 0.31 | 2.80 | 1.210 | 1.3630 |
| 0.36 | 3.35 | 1.249 | 1.3680 |
| 0.38 | 3.60 | 1.271 | 1.3706 |

Table S3: Physical parameters for sodium ethyl sulfate measured with bulk techniques. *Error on density measurements is 0.0005 g/cm³ **Error on n(589nm) measurements is 0.00005 RI units.

| Solute Mass Fraction | Molar Concentration (M) | Density* (g/cm ³) | n(589nm)** |
|----------------------|-------------------------|-------------------------------|------------|
| 0.00 | 0.00 | 0.998 | 1.3330 |
| 0.0087 | 0.071 | 1.003 | 1.3337 |
| 0.014 | 0.11 | 1.005 | 1.3343 |
| 0.018 | 0.14 | 1.007 | 1.3346 |
| 0.023 | 0.18 | 1.009 | 1.3350 |
| 0.031 | 0.25 | 1.013 | 1.3357 |
| 0.044 | 0.36 | 1.020 | 1.3368 |
| 0.055 | 0.45 | 1.025 | 1.3377 |
| 0.076 | 0.63 | 1.037 | 1.3399 |
| 0.077 | 0.63 | 1.035 | 1.3397 |
| 0.08 | 0.66 | 1.038 | 1.3402 |
| 0.09 | 0.74 | 1.043 | 1.3409 |
| 0.11 | 0.92 | 1.051 | 1.3424 |
| 0.12 | 1.00 | 1.054 | 1.3630 |
| 0.14 | 1.18 | 1.066 | 1.3452 |
| 0.16 | 1.37 | 1.077 | 1.3471 |
| 0.19 | 1.65 | 1.092 | 1.3499 |
| 0.21 | 1.84 | 1.104 | 1.3520 |
| 0.24 | 2.13 | 1.121 | 1.3550 |
| 0.30 | 2.74 | 1.153 | 1.3607 |
| 0.40 | 3.83 | 1.209 | 1.3703 |
| 0.56 | 5.82 | 1.311 | 1.3876 |

Table S4: Surface tensions of 5.5 – 10 μm radius aqueous sodium organosulfates droplets measured with holographic optical tweezers. Tabulated concentrations and surface tensions are averages and standard deviations for 0.25 M bins. Where no standard deviations are given, only a single point fell within the concentration bin.

| Sodium methyl sulfate | | Sodium ethyl sulfate | |
|-----------------------|------------------------|----------------------|------------------------|
| Concentration (M) | Surface tension (mN/m) | Concentration (M) | Surface tension (mN/m) |
| 0.18±0.03 | 67.9±1.7 | 0.21 | 68.5 |
| 0.34±0.05 | 67.5±2.2 | 0.37±0.08 | 63.6±0.8 |
| 0.66±0.06 | 68.4±0.9 | 1.18±0.05 | 59.9±1.3 |
| 0.85±0.06 | 67.2±0.6 | 1.36±0.05 | 59.6±0.9 |
| 1.08 | 66.0 | 1.65±0.04 | 59.1±0.6 |
| 1.49 | 63.5 | 1.77 | 58.5 |
| 1.62±0.07 | 65.2±1.8 | 2.05±0.04 | 57.8±0.3 |
| 1.92 | 65.3 | 2.37±0.06 | 56.3±1.8 |
| 2.09±0.07 | 66.2±1.1 | 2.63±0.04 | 56.0±0.6 |
| 2.41±0.05 | 63.4±2.9 | 2.84±0.02 | 56.8±1.6 |
| 2.60±0.04 | 62.7±1.1 | 3.12±0.11 | 54.4±0.8 |
| 2.90 | 63.4 | 5.03 | 52.1 |
| 3.09±0.04 | 61.3±1.4 | | |
| 3.44 | 58.7 | | |
| 4.23±0.02 | 59.3±1.1 | | |
| 4.55 | 55.5 | | |
| 4.92 | 58.6 | | |

Table S5: Sum square errors (a_w units) between measured water activities of sodium methyl and ethyl sulfate solutions and AIOMFAC calculations for aqueous solutions of other short alkyl chain organics.

| AIOMFAC calculation | Sodium methyl sulfate | Sodium ethyl sulfate |
|-----------------------------------|-----------------------|----------------------|
| Ethanol | 0.018 | 0.036 |
| Formic acid | 0.021 | 0.057 |
| Acetic acid | 0.014 | 0.032 |
| Propanoic acid | 0.027 | 0.043 |
| NaHSO ₄ | 0.019 | 0.072 |
| (Na) ₂ SO ₄ | 0.013 | 0.042 |

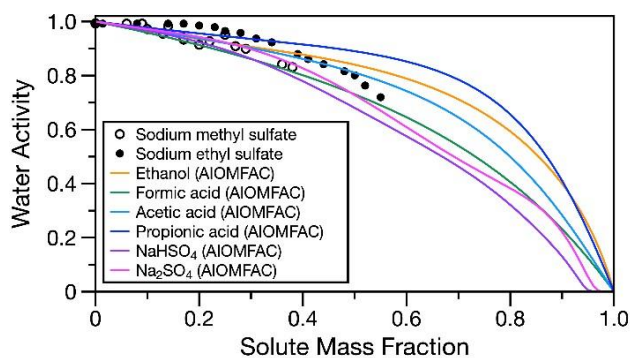


Figure S1: Comparing measured water activities for sodium methyl and ethyl sulfates to predicted water activities from AIOMFAC^{1,2} for sodium sulfate and bisulfate as well as organic molecules having similar alkyl chain lengths but with an alcohol or carboxylic acid functionality.

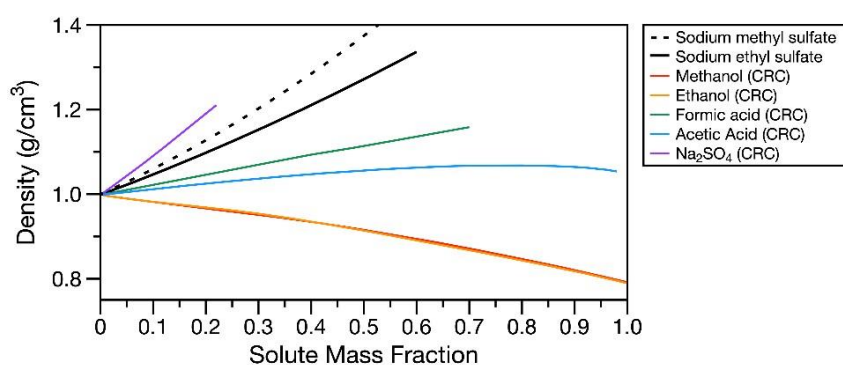


Figure S2: Comparing density parametrizations for sodium methyl and ethyl sulfates to densities from the CRC handbook³ for sodium sulfate and organic molecules having similar alkyl chain lengths but with alcohol or carboxylic acid functionality.

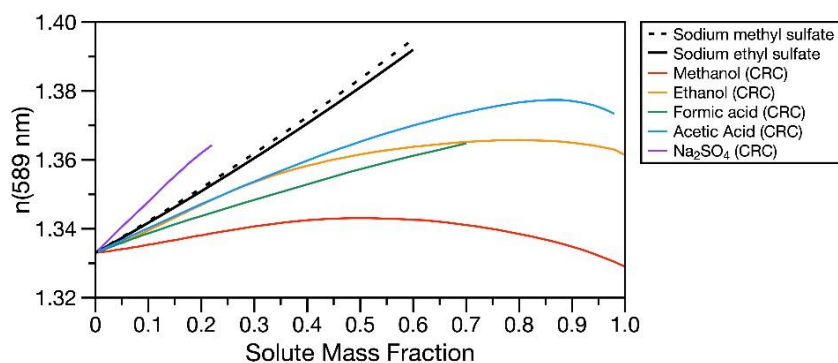


Figure S3: Comparing refractive index at 589 nm parametrizations for sodium methyl and ethyl sulfates to refractive indices from the CRC handbook for sodium sulfate and organic molecules having similar alkyl chain lengths but with alcohol or carboxylic acid functionality.

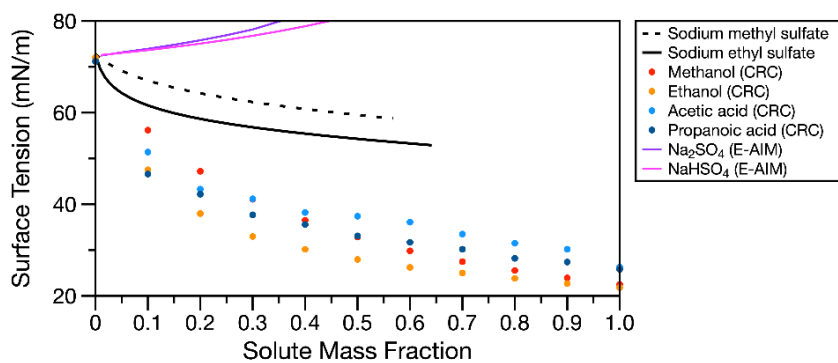


Figure S4: Langmuir isotherm fits of surface tension measurements for sodium methyl and ethyl sulfates compared to predictions for sodium sulfate and bisulfate from E-AIM^{4,5} and short alkyl chain length organics having an alcohol or carboxylic acid functional group from the CRC handbook.³

References

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