Supplemental Information for

Hygroscopicity of Isoprene-Derived Secondary Organic Aerosol Mixture Proxies: The Importance of Solute Diffusion and Salting-In Effects

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Keywords: Hygroscopicity, Organic Aerosols, IEPOX, SOA, viscosity, AFM, CCN

Contents:

I. Surface Tension Solution Concentrations

Table S1. Stock solution concentrations for dilutions.

Compound	Mass (mg)	Water (mL)	Molarity (M)
2-MT	87.1	2	0.319
2-MTS	134.7	2	0.313

Table S2. Dilutions of 2-MT solutions for surface tension measurements.

Target 2-MT Concentration (M)	Volume of 0.3 M 2-MT Stock (µL)	Volume of UPF Water (µL)
0.003	20.0	1980.0
0.005	33.3	1966.7
0.009	60.0	1940.0
0.016	106.7	1893.3
0.030	200.0	1800.0
0.094	626.7	1373.3

Table S3. Dilutions of 2-MTS solutions for surface tension measurements.

Target 2-MTS Concentration (M)	Volume of 0.3 M 2-MT Stock (µL)	Volume of UPF Water (µL)
0.003	20.0	1980.0
0.009	60.0	1940.0
0.03	200.0	1800.0
0.053	353.3	1646.7
0.094	626.7	1373.3

Table S4. Concentrations of 2-MT/AS mixture dilutions for surface tension measurements.

Target 2-MT Concentration (mM)	Target AS Concentration (mM)	Volume of 0.3 M 2-MTS Stock (µL)	Volume of 3.5 M AS Stock (µL)	Volume of UPF Water (µL)
0.003	0.5	20	285.7	1694.3
0.009	0.5	63.2	285.7	1651.1
0.03	0.5	200	285.7	1514.3
0.09	0.5	632	285.7	1082.3

Table S5. Concentrations of 2-MTS/AS mixture dilutions for surface tension measurements.

Target 2-MTS Concentration (mM)	Target AS Concentration (mM)	Volume of 0.3 M 2-MTS Stock (µL)	Volume of 3.5 M AS Stock (µL)	Volume of UPF Water (µL)
0.003	0.5	20	285.7	1694.3
0.009	0.5	63.2	285.7	1651.1
0.03	0.5	200	285.7	1514.3
0.05	0.5	355.7	285.7	1358.6

II. Experimental Solutions for Aerosol Measurements

Table S6. Solution compositions.

Mass wt% Organic (2-MT or 2-MTS sample)	Mass of Organic Sample (mg)	Mass of AS (mg)
100	10	0
90	9	1
75	7.5	2.5
60	6	4
50	5	5
40	4	6
25	2.5	7.5
10	0	10

III. H-TDMA Set Up and Calibration

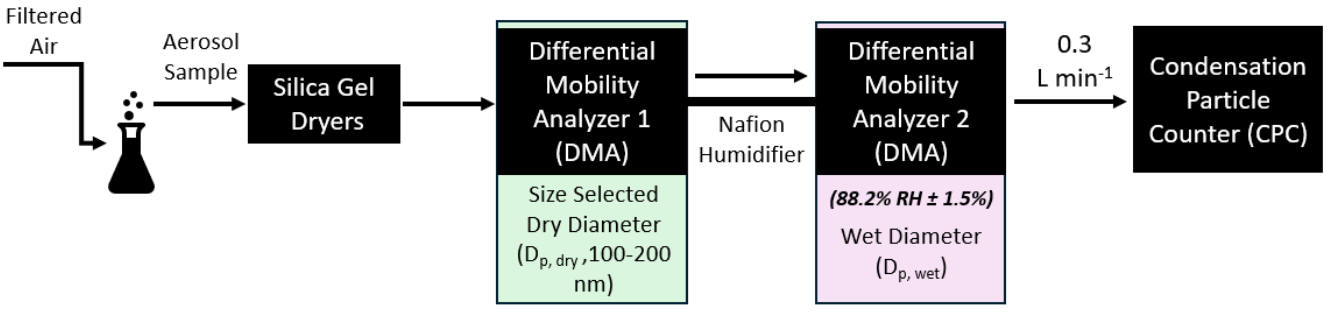

Figure S1. Experimental set up for H-TDMA measurements; dry, polydisperse aerosols were size selected through DMA1 at a 10:1 aerosol to sheath flow rate. The size selected particles are passed through a Nafion tube and humidified to 89.4% ± 2% RH. Droplet growth factor was measured using DMA2 and CPC.

Table S7. H-TDMA Ammonium Sulfate Calibration.

Size Selected Dry Diameter (nm)	Measured G_F	Relative Humidity
100	1.70	0.86
100	1.70	0.87
100	1.71	0.87
100	1.71	0.87
100	1.71	0.87
100	1.85	0.90
100	1.85	0.90
100	1.72	0.87
100	1.71	0.87
100	1.71	0.87
150	1.75	0.88
150	1.75	0.88
150	1.77	0.88
150	1.76	0.88
150	1.89	0.90
150	1.89	0.90
150	1.76	0.88
150	1.76	0.88
150	1.77	0.88
150	1.93	0.91
150	1.93	0.91

IV. CCNC Set Up and Calibration

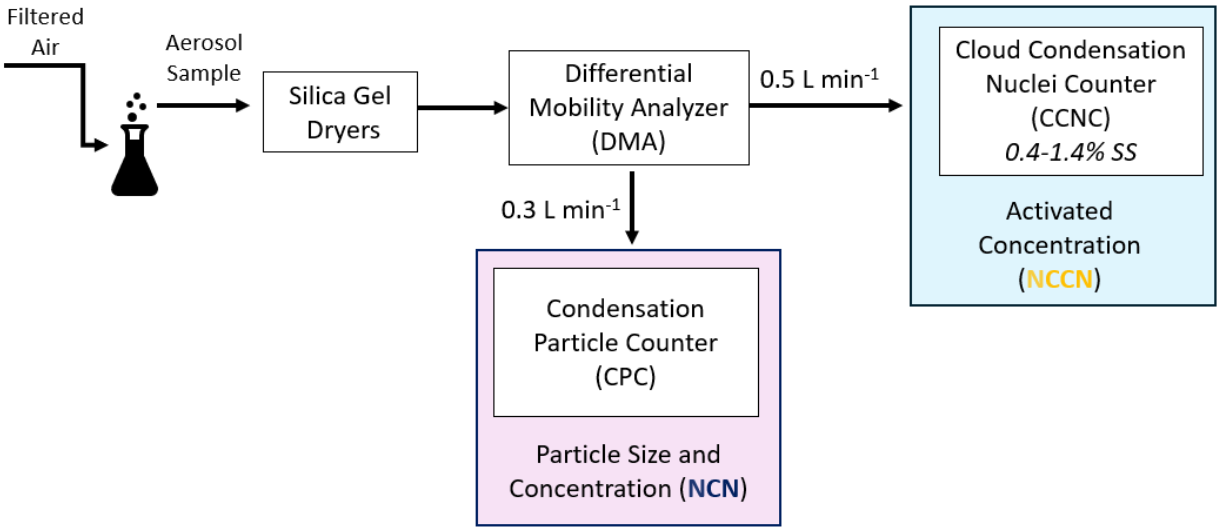

Figure S2. Experimental set up for Cloud Condensation Nuclei Counter (CCNC) experiments; dry, polydisperse aerosols were passed through the DMA at a 10:1 aerosol to sheath flow rate; aerosols were flowed into the CPC and CCN in parallel at 0.3 L min^{-1} and 0.5 L min^{-1}, respectively. The CPC was used to obtain NCN and the CCNC was used to obtain NCCN.

Table S8. CCNC Ammonium Sulfate Calibration.

Activation diameter (nm)	Calibrated supersaturation (%)
58.697	0.338
57.013	0.353
58.697	0.338
58.697	0.338
60.382	0.324
58.697	0.338
56.451	0.358
57.574	0.343
57.574	0.343
58.136	0.338
57.574	0.343
57.574	0.343
58.136	0.338
47.466	0.465
49.151	0.441
51.397	0.412

49.713	0.433
49.713	0.433
49.713	0.433
50.274	0.421
37.359	0.666
40.166	0.597
40.166	0.597
38.482	0.637
38.482	0.637
38.482	0.637
32.866	0.808
32.866	0.808
32.866	0.808
32.866	0.808
26.689	1.105
27.812	1.039
27.812	1.039
27.812	1.039
27.812	1.039
21.636	1.518
23.882	1.307
25.005	1.22
24.443	1.262
25.005	1.22
25.005	1.22
21.636	1.518
22.759	1.406
21.636	1.518
22.197	1.46
22.197	1.46
21.636	1.518
21.636	1.518
22.197	1.454

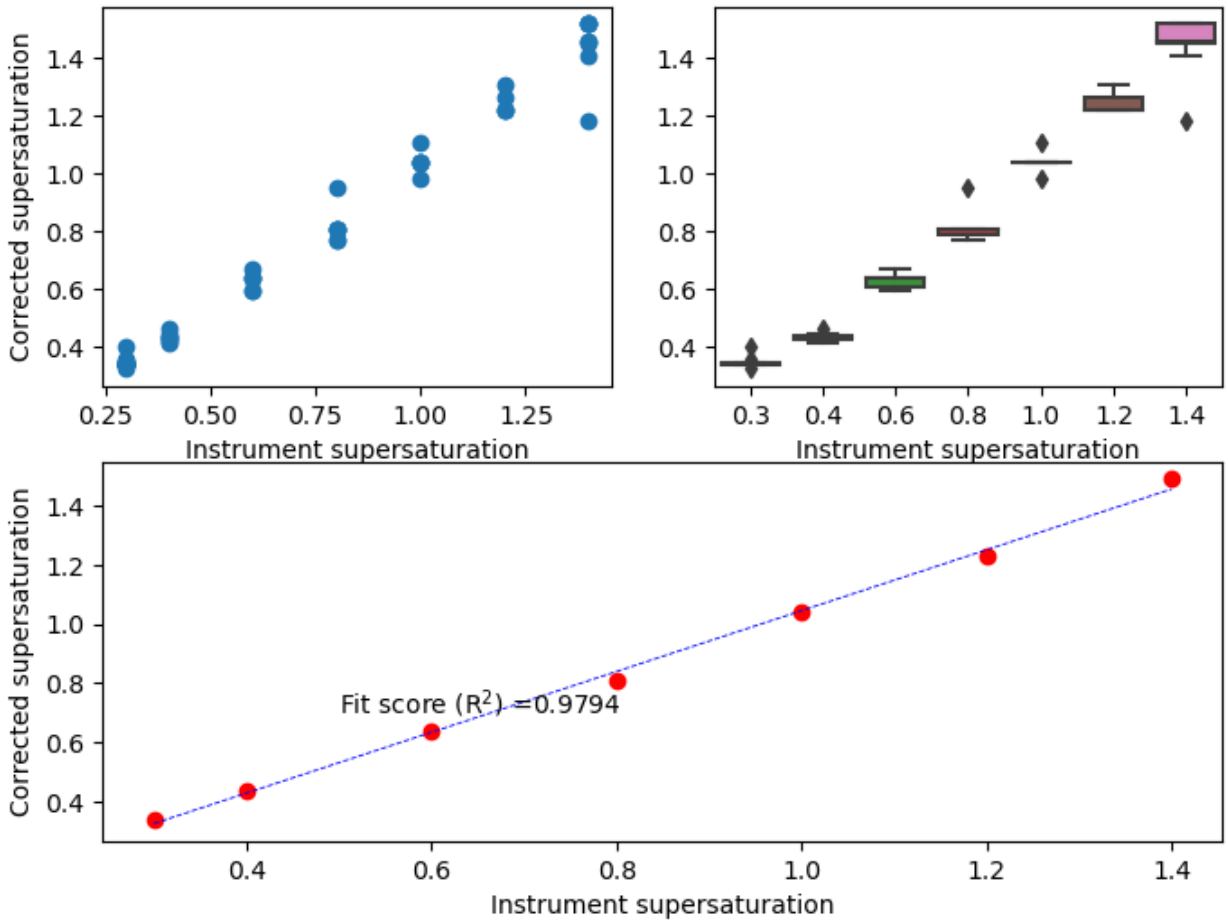

Figure S3. Ammonium sulfate (AS) CCNC instrument calibration.

V. Abbreviations

Table S9. Variable abbreviations and definitions.

Abbreviation	Definition
D_s	Organic diffusion coefficient within solvent (water) (m^2 s^{-1})
D_w	Droplet wet diameter (m)
D_d	Aerosol dry diameter (m)
$D_{p,\,50}$	Critical dry diameter size where ~50% of particles activate
SS	Supersaturation (%)
κ_{int}	Intrinsic hygroscopicity based on solute physicochemical properties
κ_{ZSR}	Mixture hygroscopicity based on ZSR mixing rule
$\kappa_{H\text{-}TDMA}$	Subsaturated hygroscopicity based on H-TDMA measurements
κ_{CCN}	Supersaturated hygroscopicity based on CCNC measurements

VI. Surface Tension Results

Table S10. Average Surface Tension Results for 2-MT, 2-MTS, and mixtures with 500 mM AS.

	Average Surface Tension (mN m^{-1})			
Sample Concentration (mM)	**2-MT**	**2-MT/AS w/ 500 mM AS**	**2-MTS**	**2-MTS/AS w/ 500 mM AS**
3	72.048 ± 0.130	75.296 ± 0.108	73.027± 0.035	75.131 ± 0.246
5	71.753 ± 0.029			
9	73.512 ± 1.242	74.942 ± 0.360	72.184 ± 0.012	72.912 ± 0.177
16	72.321 ± 0.036			
30	70.713 ± 0.479	74.314 ± 0.430	71.426 ± 0.067	72.514 ± 0.144
53			69.835 ± 0.124	74.177 ± 0.173
94	71.279 ± 0.004	72.109 ± 0.067	67.950 ± 0.241	

Table S11. Sodium Ethyl Sulfate Surface Tension Measurements from Peng et al., 2016.

Solute Concentration (M)	Average Surface Tension (mN m^{-1})	Std Dev
0.001	76.329	0.199
0.002	75.805	0.372
0.003	75.212	0.188
0.007	74.789	0.119
0.010	74.460	0.131
0.014	74.090	0.089
0.017	73.668	0.203
0.020	72.970	0.198
0.024	73.248	0.446
0.030	73.729	0.264

Table S12. Sodium Methyl Sulfate Surface Tension Measurements from Peng et al., 2016.

Solute Concentration (M)	Average Surface Tension (mN m^{-1})	Std Dev
0.001	75.212	0.341
0.002	74.967	0.412
0.004	74.768	0.508
0.007	74.142	0.368
0.011	73.004	0.347
0.015	72.540	0.782
0.019	71.618	0.433
0.022	73.896	0.374
0.026	72.411	0.446
0.030	72.744	0.533
0.034	73.354	0.577

Table S13. 2-methylglutaric Acid Surface Tension Measurements from Ferdousi-Rokib et al., 2025 (in review).

Solute Concentration (M)	Average Surface Tension (mN m^{-1})	Std Dev
0.003	68.056	0.435
0.003	68.446	0.112
0.007	68.699	0.491
0.009	67.621	0.628
0.014	67.899	0.835

Table S14. Sodium Octyl Sulfate Surface Tension Measurements from Peng et al., 2016.

Solute Concentration (M)	Average Surface Tension (mN m^{-1})	Std Dev
0.000	74.210	1.197
0.001	73.161	0.964
0.002	72.159	0.789
0.004	70.761	0.674
0.006	70.947	0.334
0.009	71.238	0.349
0.011	69.119	0.312
0.013	67.416	0.062
0.015	66.515	0.155
0.019	65.908	0.374
0.022	64.825	0.166
0.024	63.173	0.106
0.026	62.085	0.114

Table S15. Sodium Doedcyl Sulfate Surface Tension Measurements.

Solute Concentration (M)	Average Surface Tension (mN m^{-1})	Std Dev
0.001	70.983	0.395
0.001	65.885	0.832
0.002	65.945	0.359
0.003	63.815	0.240
0.003	61.186	0.406
0.003	58.065	0.328
0.004	48.992	0.442
0.005	46.791	0.313
0.006	46.715	0.526
0.007	44.460	0.523
0.009	39.464	0.385
0.010	38.905	0.097
0.010	39.942	0.075
0.014	39.919	0.064
0.017	39.347	0.047
0.021	39.157	0.049
0.024	38.816	0.049
0.028	39.190	0.030
0.031	39.165	0.052
0.035	38.917	0.032

Table S16. Ammonium Sulfate Surface Tension Measurements from Ferdousi-Rokib et al., 2025 *(in review).*

Solute Concentration (M)	Average Surface Tension (mN m^{-1})	Std Dev
0.015	71.993	0.222
0.009	70.482	0.622
0.008	70.032	0.303
0.004	71.517	0.221
0.003	70.690	0.227

VII. Diffusion Coefficients and Viscosities

Table S17. Diffusion coefficients of 2-MT and 2-MTS in water and aqueous mixture with 500 mM AS.

	Diffusion Coefficient (m^2 s^{-1})			
Sample Concentration (mM)	**2-MT**	**2-MT/AS w/ 500 mM AS**	**2-MTS**	**2-MTS/AS w/ 500 mM AS**
3	1.03E-09	8.53E-09	3.88E-09	6.57E-09
5	4.83E-09			
9	2.15E-10	7.72E-10	1.45E-10	7.7E-09
16	2.43E-10			
30	4.72E-10	1.43E-10	1.37E-10	2.75E-09
53			1.63E-10	3.88E-09
94	1.39E-11	1.091E-10	1.04E-10	

Table S18. Estimated Viscosity of 2-MT and 2-MTS at Different Conditions

	H-TDMA	**Before Entering the CCNC**
2-MT	0.27-0.63	8.9E4
2-MTS	22-14	3.1E8

Table S19. Estimated Diffusion Coefficient of 2-MT and 2-MTS at Different Conditions

Diffusion (cm^2 s^{-1})	**H-TDMA**	**Before Entering the CCNC**
2-MT	3.5-8.1 E-8	2.5E-13
2-MTS	1.6-4.9 E-8	1.2E-16

VIII. Information on Additional Compounds

Table S20. Calibration and compound information for additional compounds

Compound	Molecular Weight (g mol^{-1})	Density (g cm^{-3})	Average surface tension (mN m^{-1})	κ
Ammonium Sulfate ($(NH_4)_2SO_4$)	132.14[a]	1.77[a]	73.8	0.61
Sodium Methyl Sulfate (CH_3NaO_4S)	134.08[$]	1.60[$]	72.80[$]	0.459[$]

[a]Sigma Aldrich
[$]Peng et al 2021

Table S21. Adjusted mass wt% of organic based on impurities

Mass wt% Organic (2-MTS sample)	**Mass wt% of Pure 2-MTS**
90	65.7
75	54.75
60	43.8
50	36.5
40	29.2
25	18.25
10	7.3

IX. Subsaturated Hygroscopicity Results

Table S22. Growth factor and subsaturated hygroscopicity results for 2-MT and 2-MT/AS mixtures.

Mass wt% 2-MT	D_{dry} (nm)	GF	StdDev	κ	StdDev
100	100	1.396	0.002	0.076	0.002
	150	1.419	0.004	0.106	0.003
	200	1.436	0.006	0.128	0.005
90	100	1.518	0.001	0.353	0.001
	150	1.534	0.002	0.369	0.002
	200	1.561	0.001	0.396	0.001
75	100	1.614	0.001	0.453	0.001
	150	1.636	0.000	0.477	0.001
	200	1.650	0.004	0.494	0.004
60	100	1.717	0.002	0.482	0.002
	150	1.702	0.002	0.466	0.002
	200	1.715	0.003	0.479	0.003
50	100	1.625	0.002	0.500	0.002
	150	1.625	0.009	0.500	0.011
	200	1.643	0.002	0.523	0.002
40	100	1.689	0.002	0.586	0.003
	150	1.705	0.001	0.606	0.002
	200	1.699	0.003	0.598	0.004
25	100	1.809	0.003	0.602	0.003
	150	1.808	0.002	0.601	0.002
	200	1.839	0.003	0.587	0.003
10	100	1.877	0.000	0.608	0.004
	150	1.872	0.027	0.627	0.007
	200	1.859	0.000	0.623	0.004

Table S23. Growth factor and subsaturated hygroscopicity results for 2-MTS and 2-MTS/AS mixtures.

Mass wt% 2-MTS	D_{dry} (nm)	GF	StdDev	κ	StdDev
100	100	1.455	0.003	0.134	0.004
	150	1.538	0.007	0.250	0.010
	200	1.588	0.022	0.326	0.005
65.7	100	1.538	0.003	0.356	0.003
	150	1.625	0.004	0.403	0.004
	200	1.625	0.005	0.445	0.005
54.8	100	1.560	0.001	0.389	0.001
	150	1.605	0.003	0.435	0.003
	200	1.641	0.001	0.476	0.001
43.8	100	1.674	0.001	0.513	0.001
	150	1.694	0.008	0.566	0.010
	200	1.730	0.001	0.592	0.001
36.5	100	1.702	0.001	0.546	0.001
	150	1.746	0.005	0.581	0.000
	200	1.771	0.004	0.581	0.000
29.2	100	1.747	0.011	0.602	0.000
	150	1.730	0.003	0.581	0.000
	200	1.794	0.006	0.501	0.000
18.25	100	1.811	0.000	0.529	0.008
	150	1.846	0.026	0.584	0.004
	200	1.860	0.042	0.598	0.009
7.30	100	1.868	0.001	0.580	0.001
	150	1.917	0.001	0.583	0.001
	200	1.933	0.008	0.600	0.008

X. Supersaturated Hygroscopicity Results

Table S24. Supersaturated hygroscopicity results for 2-MT and 2-MT/AS mixtures.

Mass wt% 2-MT	Instrument SS	$D_{p,50}$	StdDev	κ	StdDev
100	0.318	81.300	1.337	0.102	0.020
	0.43	67.832	1.888	0.086	0.027
	0.653	50.528	0.852	0.105	0.018
	0.876	41.218	0.722	0.105	0.019
	1.099	34.767	0.000	0.138	0.000
	1.323	29.928	0.000	0.171	0.000
	1.546	25.694	1.075	0.221	0.029
90	0.324	75.859	1.294	0.300	0.016
	0.427	62.040	0.693	0.316	0.010
	0.633	46.810	2.240	0.341	0.061
	0.839	38.638	0.866	0.343	0.023
	1.045	32.831	0.000	0.360	0.000
	1.251	27.412	0.474	0.433	0.022
	1.458	23.517	0.469	0.505	0.030
75	0.324	72.509	0.930	0.344	0.014
	0.427	60.412	0.780	0.342	0.014
	0.633	45.950	1.031	0.355	0.022
	0.839	36.702	0.000	0.398	0.000
	1.045	29.928	0.000	0.475	0.000
	1.251	27.267	0.419	0.439	0.020
	1.458	23.431	0.437	0.511	0.028
60	0.324	63.155	0.994	0.520	0.023
	0.427	52.626	0.482	0.517	0.016
	0.633	40.036	0.663	0.536	0.027
	0.839	33.799	0.866	0.512	0.039
	1.045	28.315	0.456	0.561	0.026
	1.251	25.283	0.387	0.551	0.024
	1.458	22.186	0.000	0.601	0.000
50	0.324	63.509	0.619	0.517	0.020
	0.427	53.584	1.217	0.495	0.034
	0.633	41.541	0.838	0.486	0.026
	0.839	34.961	0.387	0.470	0.015
	1.045	29.283	0.456	0.517	0.024
	1.251	26.057	0.000	0.512	0.000
	1.458	22.463	0.437	0.591	0.033
40	0.324	60.808	0.964	0.581	0.031
	0.427	51.509	0.619	0.550	0.019
	0.633	40.670	0.677	0.509	0.026
	0.839	33.993	0.387	0.501	0.017

	1.045	29.928	0.000	0.473	0.000
	1.251	26.057	0.000	0.502	0.000
	1.458	22.401	0.402	0.583	0.030
25	0.324	60.654	0.640	0.585	0.017
	0.427	50.735	0.484	0.577	0.014
	0.633	40.397	0.556	0.521	0.023
	0.839	34.041	0.803	0.499	0.036
	1.045	28.960	0.000	0.524	0.000
	1.251	25.250	0.361	0.553	0.023
	1.458	23.033	0.320	0.537	0.022
10	0.324	59.848	1.004	0.610	0.031
	0.427	50.832	0.474	0.573	0.017
	0.633	40.159	0.479	0.530	0.018
	0.839	32.831	0.000	0.555	0.000
	1.045	28.960	0.000	0.522	0.000
	1.251	25.283	0.387	0.550	0.024
	1.458	22.831	0.456	0.551	0.034

Table S25. Supersaturated hygroscopicity results for 2-MT and 2-MT/AS mixtures.

Mass wt% 2-MTS	Instrument SS	$D_{p,50}$	StdDev	κ	StdDev
100.0	0.318	78.688	1.289	0.164	0.020
	0.430	65.654	1.830	0.135	0.028
	0.653	49.864	1.313	0.132	0.027
	0.876	42.348	0.361	0.102	0.010
	1.099	35.735	0.000	0.123	0.000
	1.323	30.702	1.129	0.143	0.032
	1.546	27.872	0.320	0.151	0.015
65.7	0.318	73.638	0.954	0.342	0.015
	0.430	61.248	0.622	0.325	0.011
	0.653	47.670	0.456	0.299	0.008
	0.876	39.606	0.000	0.292	0.000
	1.099	32.638	0.387	0.333	0.012
	1.323	29.202	0.419	0.321	0.013
	1.546	26.178	0.320	0.327	0.011
54.8	0.318	72.286	1.084	0.364	0.016
	0.430	59.638	1.064	0.353	0.016
	0.653	47.133	0.402	0.312	0.008
	0.876	38.396	0.419	0.325	0.011
	1.099	33.799	0.000	0.303	0.000
	1.323	28.960	0.000	0.333	0.000
	1.546	25.694	0.674	0.351	0.026
43.8	0.318	67.231	0.634	0.446	0.011
	0.430	56.585	1.041	0.410	0.022
	0.653	44.251	0.843	0.372	0.021
	0.876	35.735	0.000	0.395	0.000
	1.099	30.896	0.000	0.389	0.000
	1.323	27.025	0.000	0.402	0.000
	1.546	24.122	0.000	0.415	0.000
36.5	0.318	66.461	1.318	0.459	0.029
	0.430	56.272	0.608	0.412	0.011
	0.653	44.030	0.874	0.377	0.020
	0.876	35.735	0.000	0.394	0.000
	1.099	31.283	0.474	0.374	0.017
	1.323	27.025	0.000	0.401	0.000
	1.546	23.517	0.469	0.448	0.026
29.2	0.318	63.638	1.415	0.523	0.032
	0.430	53.832	0.620	0.472	0.019
	0.653	41.420	0.756	0.450	0.026
	0.876	34.961	0.022	0.418	0.022
	1.099	29.154	0.387	0.462	0.018
	1.323	26.057	0.000	0.447	0.000

	1.546	22.428	0.419	0.515	0.027
18.3	0.318	64.203	1.149	0.517	0.025
	0.430	52.802	0.622	0.508	0.021
	0.653	42.785	1.123	0.418	0.029
	0.876	34.767	0.000	0.436	0.000
	1.099	29.686	0.803	0.447	0.035
	1.323	26.057	0.000	0.456	0.000
	1.546	22.186	0.000	0.542	0.000
7.3	0.318	59.840	0.767	0.632	0.024
	0.430	51.219	0.433	0.553	0.013
	0.653	40.358	0.887	0.491	0.033
	0.876	32.831	0.000	0.510	0.000
	1.099	29.154	0.387	0.464	0.018
	1.323	25.089	0.000	0.503	0.000
	1.546	22.186	0.000	0.534	0.000

XI. Goodness of Fit

Table S26. Köhler Theory R^2.

	κ_{ZSR} R^2	
Mixture	**H-TDMA**	**CCN**
2-MT/AS	0.686	0.787
2-MTS/AS	0.913	0.972

XII. Additional AFM Figures

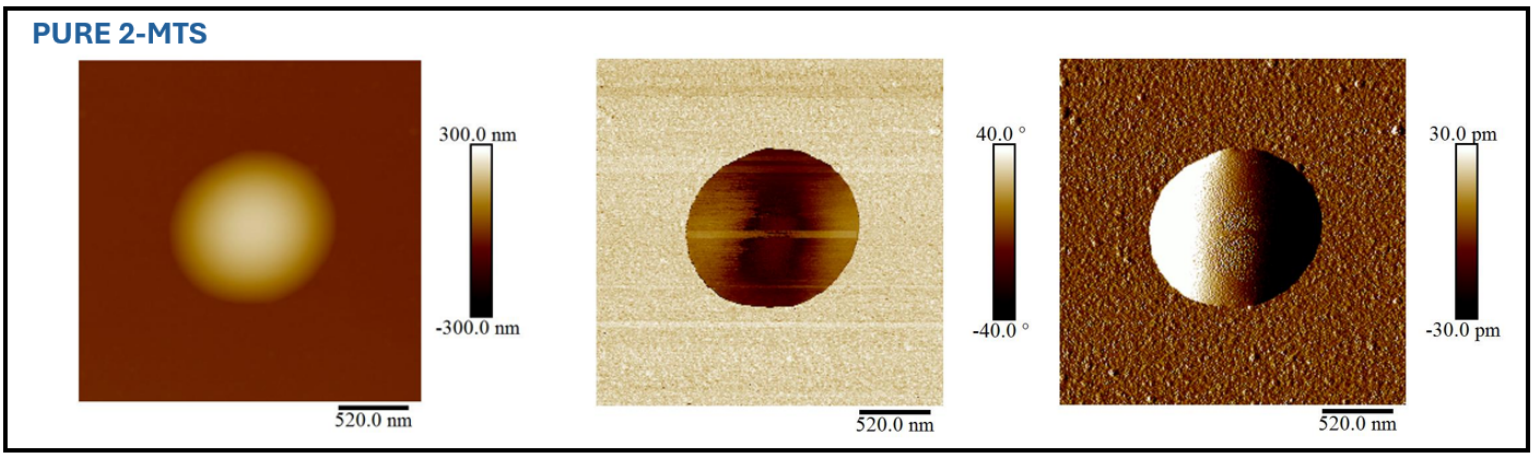

Figure S4. AFM Image of 100wt% synthesized 2-MTS and visualization. The figure shows the height, phase, and amplitude error from left to right.

XIII. 2-MT D_d vs κ_{CCN}

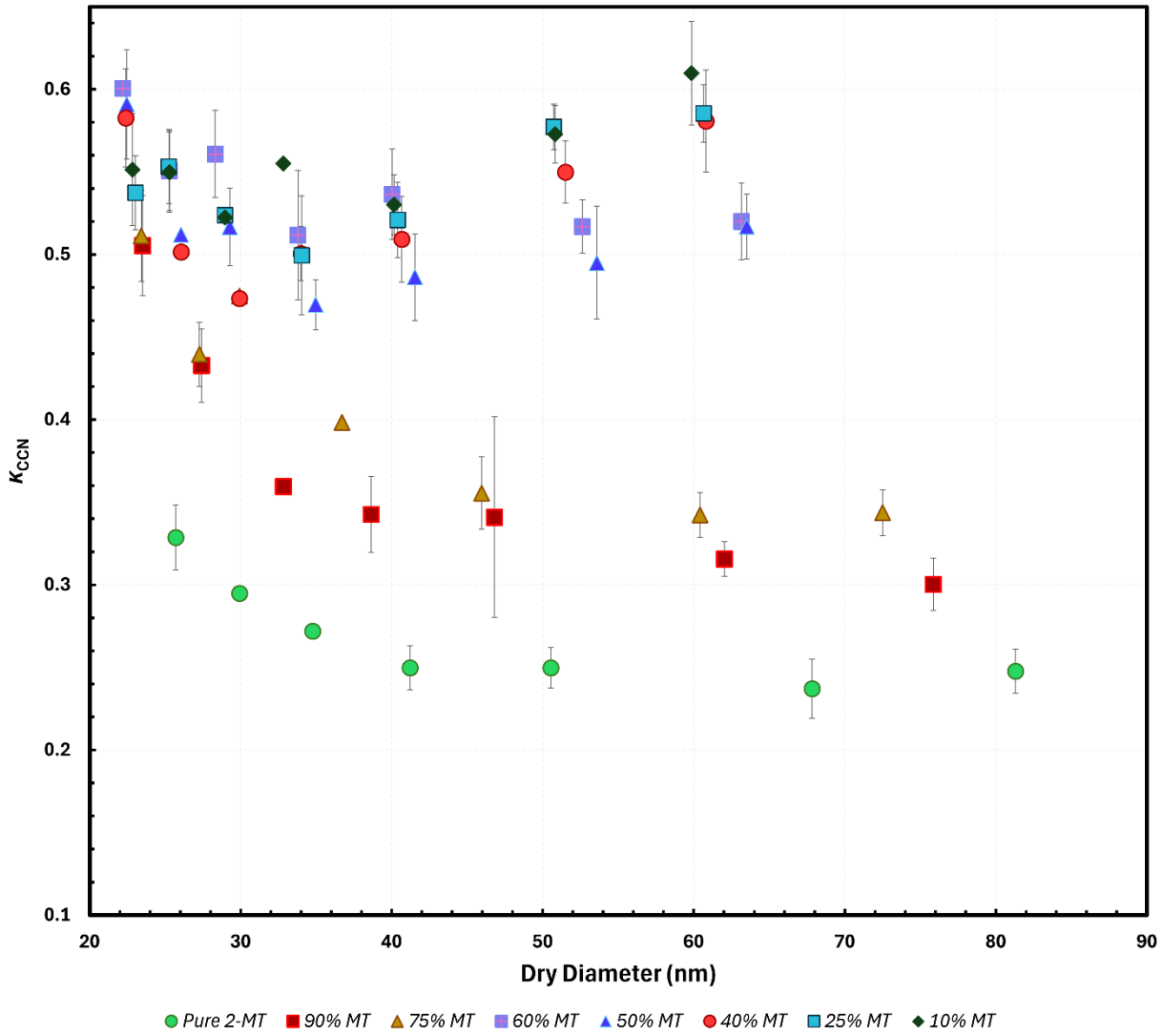

Figure S5. 2-MT D_d vs κ_{CCN} of all mixtures and 100 wt% 2-MT aerosols.