Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Information for

Integrated Experimental and Theoretical Approach to Probe the Synergistic Effect of Ammonia in Methanesulfonic Acid Reactions with Small Alkylamines

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Environmental Science: Processes and Impacts

1. Description of the two flow tube reactors used in this study.

MSA + MA system. Figure 1a is a schematic of the flow reactor used for the MA studies. The sequence of addition of the different reactants is described below. A total of ~13 L min^{-1} of dry clean air was injected in the first ring (ring A). RH conditions investigated ranged from RH < 3% (dry conditions) up to ~ 45-50% (corresponding to a H_2O concentration of ~3×10^{17} molecules per cm^3 at T = 296 K). For those, a fraction of the flow was diverted to a bubbler filled with nanopure water (Barnstead, 18.2 MΩ-cm; Thermo model 7146) and mixed with the remaining of dry air before being introduced through ring A. No air flow was introduced through ring B and C. When present, NH_3 was mixed in with clean dry air and injected through the first spoked inlet (spoke 1) to yield a total flow rate of 1 L min^{-1} through spoke 1. MSA (~0.1 L min^{-1} over the pure liquid maintained in a glass trap at room temperature) was mixed with ~1.9 L min^{-1} of clean dry air and the mixture introduced through the second spoked inlet (spoke 2). MA (~0.2 L min^{-1} from the permeation tube) was mixed in with ~0.8 L min^{-1} of clean dry air and added through the third spoked inlet (spoke 3). The total flow rate through the flow reactor under those conditions was ~17 L min^{-1}. All flows were controlled by high-precision mass flow controllers (Alicat or MKS) and were checked with a flow meter (Gilibrator 2, Sensidyne) before each experiment. Note that the perforations located on spoke 3 are facing backward which provides good mixing of the MA with MSA and NH_3. Total particle concentrations (N_{total}, particles per cm^3) and size distributions of the particles as a function of reaction time were measured by moving the sampling line away from the spoked inlets, corresponding to reaction times 0.4 s, 1.6 s, 2.9 s, 4.2 s and 5.3 s with respect to the MSA injection port, based on a conversion factor from previous measurements.[1] Note that the time travelled in the sampling tube (1.9 - 3.3 s) was not included in the reaction time as it was

assumed that reactions are quenched rapidly in the sampling lines due to wall uptake of any remaining MSA or amines.

MSA + TMA system. Figure 1b is a schematic of the flow reactor conditions representative of the MSA + TMA (± NH_3) experiments. The sequence of addition of the reactants is similar to that of the MSA + MA system. However, because the MSA + TMA experiments were performed on a different flow reactor equipped with only 2 ring inlets and 2 spoked inlets, the NH_3 was added at the upstream end (ring B), while both MSA (~0.2 L min^{-1} mixed in with ~1.8 L min^{-1} of dry clean air) and TMA (~0.2 L min^{-3} from the permeation tube mixed in with ~0.8 L min^{-1} of dry clean air) were added at the spoked inlet (spokes 2 and 3 respectively). The total flow rate through the flow reactor under these conditions was ~17 L min^{-1}. Total particle concentrations (N_{total}, particles per cm^3) and size distributions of the particles formed were collected by moving the sampling line away from the spoked inlets, corresponding to reaction times 0.3 s, 1.7 s, 3.1 s, 4.5 s and 5.9 s with respect to the MSA injection port, estimated using a conversion factor based upon previous measurements.[2]

2. Comparison between the CPC and the PSM+CPC combination measurements.

The combination of the CPC with a continuous flow mixing diethylene glycol-based PSM extended the d_{50} cut-off size particle measurement from 2.5 nm (TSI; sucrose particles) down to ~1.4 nm (ammonium sulfate particles).[3] True cut-off sizes for both the CPC and PSM strongly depend of the chemical composition of the particles sampled.[3-8] The cut-off size for MSA + amine particles is not known, thus the cut-off defined for the reference compounds is applied here. The settings of the PSM were the factory settings with which the manufacturer did the calibration and are as follows: growth fluid, diethylene glycol (Sigma; ≥99.0%); growth tube

temperature, 4˚C; saturator temperature, 85˚C; fixed mode with saturator flow rate of 1 L clean dry air min^{-1}; total sample inlet flow, 2.5 L min^{-1}. Under these conditions, the detection efficiencies or cut-off diameters specified by the manufacturer for negatively charged ammonium sulfate are 1.2 nm (d_{10}), 1.4 nm (d_{50}) and 2.1 nm (d_{80}), which are the diameters at which 10%, 50% and 80% of particles are detected respectively. In order to be able to compare directly with CPC measurements, the flow through the flow reactor sampling line was kept at 1.5 L min^{-1}, and an additional 1 L min^{-1} of filtered room air was added at the entrance of the PSM.

Figure S1 and S2 compare the results of total number concentration (N_{total}, particles per cm^3) measurements using the CPC and those using the combined PSM + CPC for each system. Under dry conditions, the discrepancy between the two measurements is the largest for the MSA + MA system (smallest particles measured in the present study), and it is more pronounced at shorter reaction times. In general, the measurements are in much better agreement under high relative humidity, which is also where the particles were observed to be larger. The discrepancy was systematically observed as a decrease in N_{total} from the PSM + CPC combination compared to the CPC data. This suggests that either there were no particles of that size, or losses of the small particles were higher for the combination measurements, or that DEG was not as effective in activating these types of particles.

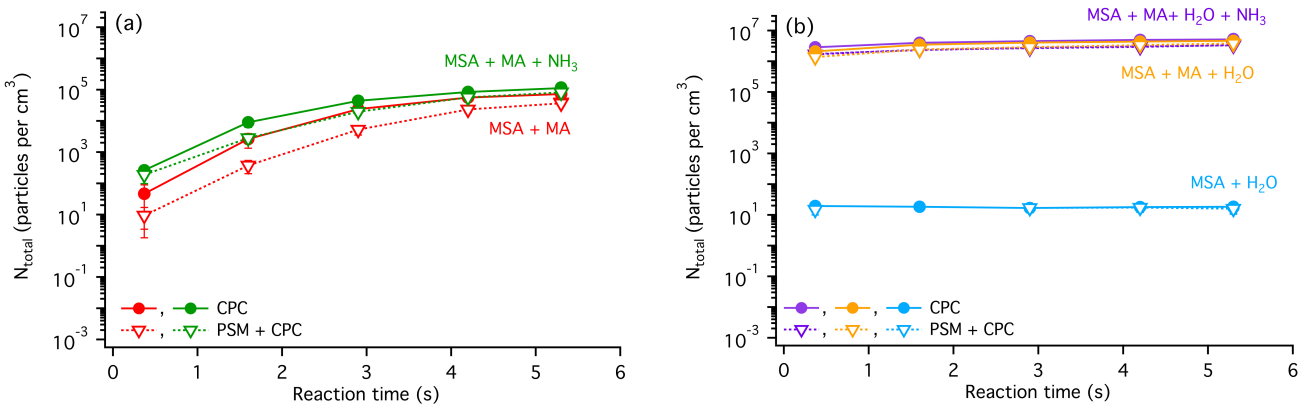

Figure S1. Total particle number concentrations (N_{total}) from the MSA + MA and MSA + MA + NH_3 reactions as a function of reaction time measured using the CPC and the PSM + CPC combination for (a) dry conditions and (b) at ~45-50% RH. Each data point corresponds to the average N_{total} measured over a 5-min scan (error bars correspond to 1 standard deviation). Concentrations of reactants are [MSA] = 6.4×10^{10} molecules per cm^3; [MA] = 6.1×10^{10} molecules per cm^3; [NH_3] = 0 or 2.9×10^{11} molecules per cm^3. Note that the data in (b) (MSA + MA + H_2O and MSA + MA + H_2O + NH_3) are corrected for dilution.

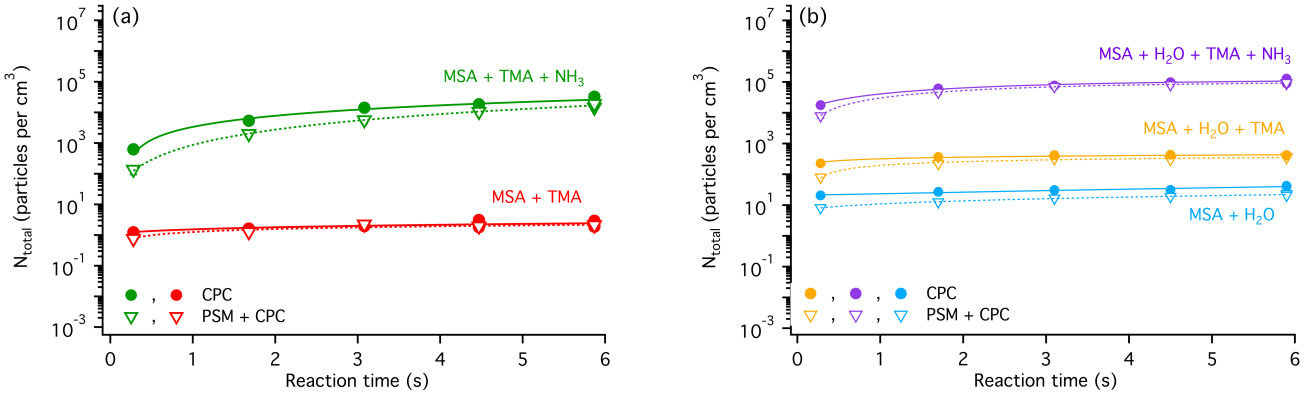

Figure S2. Total particle number concentrations (N_{total}) from the MSA + TMA and MSA + TMA + NH_3 reactions as a function of reaction time measured using the CPC and the PSM + CPC combination for (a) dry conditions and (b) at ~45-50% RH. Each data point corresponds to the average N_{total} measured over a 5-min scan (error bars correspond to 1 standard deviation). Concentrations of reactants are [MSA] = 7.9×10^{10} molecules per cm^3; [TMA] = 5.0×10^{10} molecules per cm^3; [NH_3] = 0 or 2.2×10^{10} molecules per cm^3.

3. Influence of the sheath air flow relative humidity on size distribution measurements for MSA + TMA particles (RH ~46%).

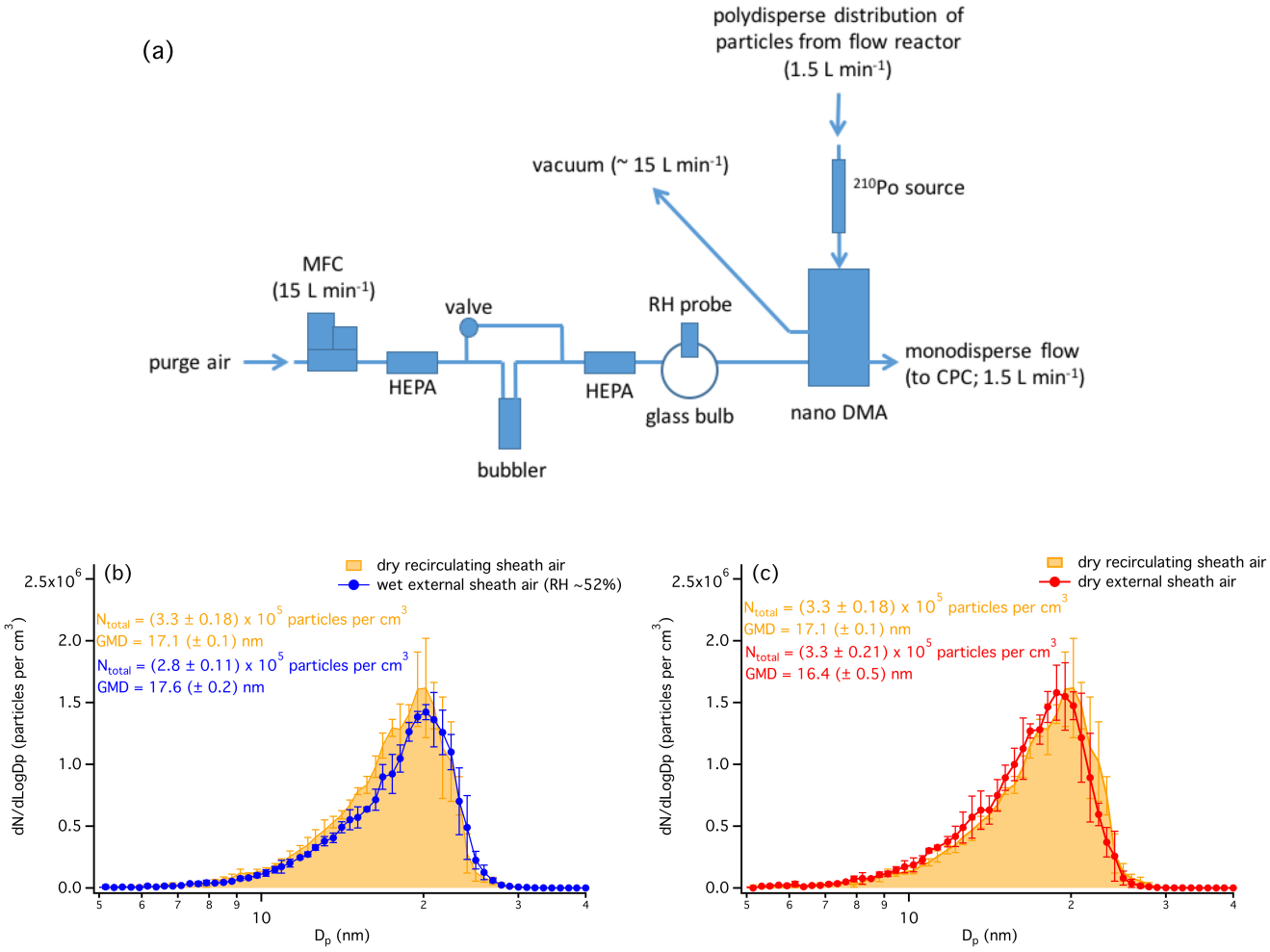

Figure S3. (a) Schematic of the SMPS configured with an external humidifier system. Size distributions measured with (b) humid sheath air (RH ~52%; blue trace) or (c) dry air (red trace, external sheath air). In both graphs, the orange trace corresponds to the normal operating conditions with recirculating dry sheath air. Each size distribution represents an average over three replicate measurements (± 1 standard deviation). Concentration of the reactants are [MSA] = 7.9×10^{10} molecules per cm^3 and [TMA] = 5.0×10^{10} molecules per cm^3.

4. MSA + MA (± NH_3) - excess MSA conditions.

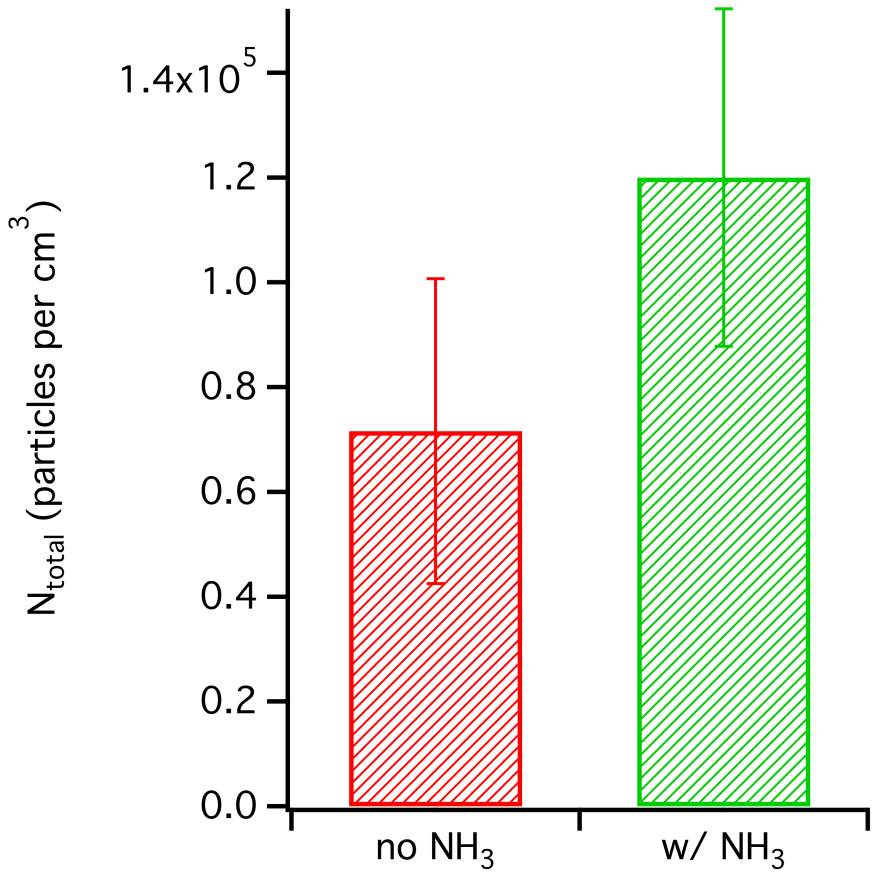

Figure S4. Total particle number concentrations (N_{total}) for the MSA + MA reaction (excess MSA conditions) measured using the CPC with or without NH_3 at t = 5.3 s. Each bar corresponds to an average taken from replicate measurements over 4 consecutive days. Concentrations of the reactants are [MSA] = 4.6×10^{10} molecules per cm^3; [MA] = 2.3×10^{10} molecules per cm^3; [NH_3] = 0 or 1.1×10^{11} molecules per cm^3.

5. Total particle number concentration from the MSA + MA and MSA + NH_3 reactions measured at 5.3 s as a function of the amine concentration under dry and humid conditions.

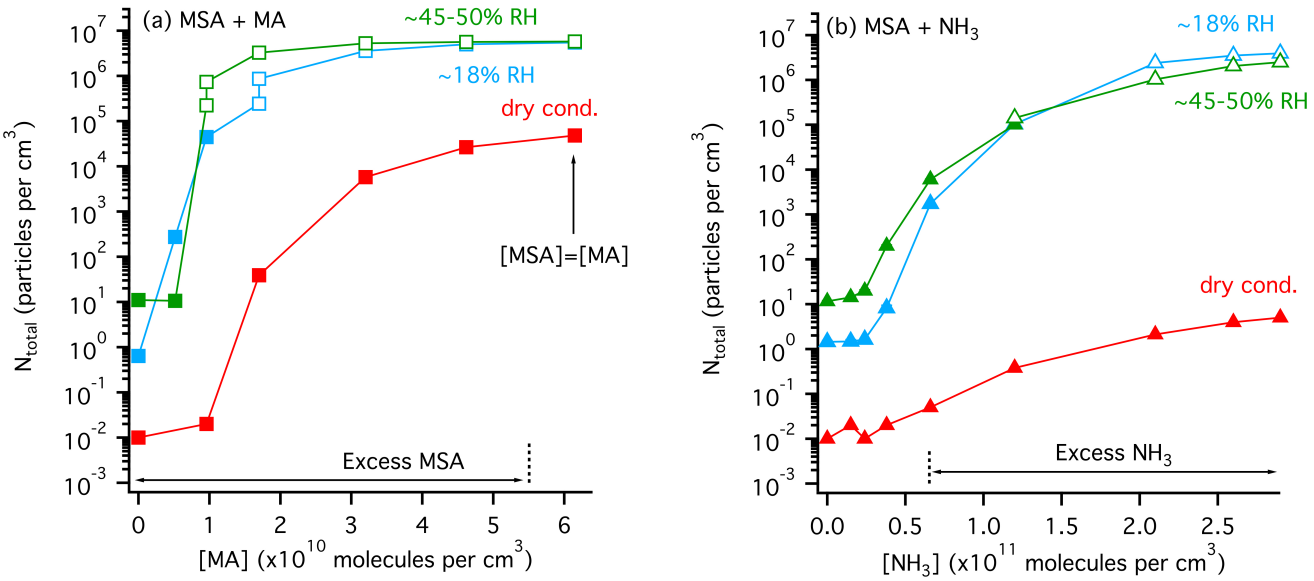

Figure S5. Total particle concentrations (N_{total}) measured using the CPC taken at 5.3 s as a function of either (a) MA or (b) NH_3 concentrations in the flow reactor (with [MSA] = 6.4×10^{10} molecules per cm^3) under dry conditions (red traces) and humid conditions (~18% RH; light blue traces; ~45-50% RH; green traces). MSA (spoke 2) and MA (spoke 3) were added to the flow reactor as shown in Fig. 1; however, for the (MSA + NH_3) system, the NH_3 was added through ring C upstream instead of spoke 1. Each data point corresponds to the average N_{total} measured from five replicate CPC measurements ±1 standard deviation), each made over 2 min. Open symbols correspond to measurements performed using a dilution system prior to the inlet of the instrument (dilution factor 25-30). The solid symbols correspond to measurements performed without dilution.

6. Determination of particle formation rates ($J_{>2.0nm}$) for MSA + MA reaction systems

6.1. MSA + MA (± NH_3), dry conditions.

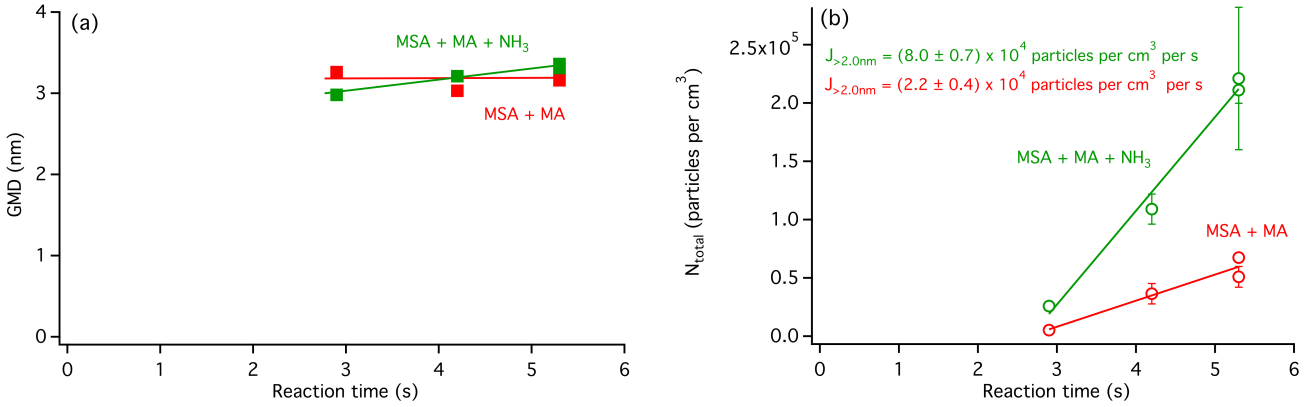

Figure S6. (a) Mobility geometric mean diameters (GMD, nm) determined from the size distributions collected as a function of reaction time for MSA + MA (red trace) and the MSA + MA + NH_3 (green trace) respectively. (b) Total particle number concentrations (N_{total}) measured using the SMPS as a function of reaction time. Each data point corresponds to the average N_{total} measured from five successive scans ± 1 standard deviation. Concentrations of the reactants are [MSA] = 6.4×10^{10} molecules per cm^3; [MA] = 6.1×10^{10} molecules per cm^3; [NH_3] = 0 or 2.9×10^{11} molecules per cm^3.

6.2. MSA+MA (± NH_3), ~45-50% RH

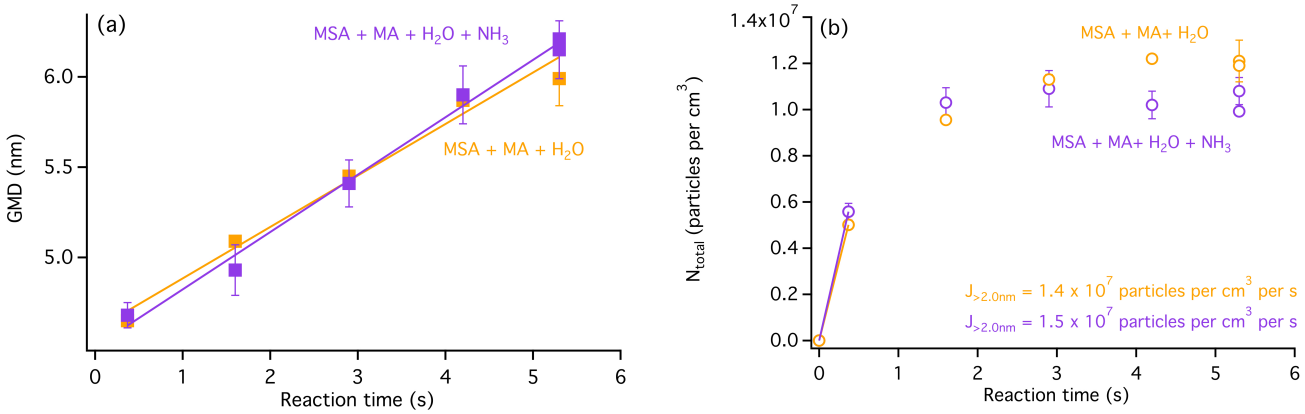

Figure S7. (a) Mobility geometric mean diameters (GMD, nm) determined from the size distributions collected as a function of reaction time for the MSA + MA + H_2O (orange trace) and the MSA + MA + H_2O + NH_3 (purple trace) respectively. (b) Total particle number concentration (N_{total}) measured using the SMPS as a function of reaction time. Each data point corresponds to the average N_{total} measured from five successive scans ± 1 standard deviation. Concentrations of the reactants are [MSA] = 6.4×10^{10} molecules per cm^3; [MA] = 6.1×10^{10} molecules per cm^3; [NH_3] = 0 or 2.9×10^{11} molecules per cm^3.

7. Size distribution comparison for MSA + H_2O + NH_3, MSA + H_2O + MA, MSA + H_2O + MA + NH_3 reaction systems.

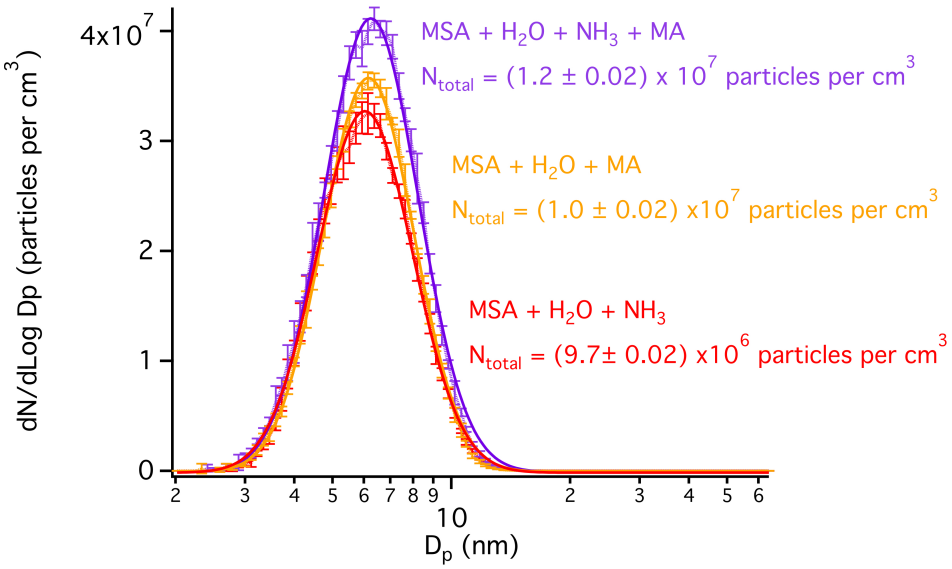

Figure S8. Size distributions acquired at a reaction time of 5.3 s for MSA + H_2O + NH_3 (red trace), MSA + H_2O + MA (orange trace), and MSA + H_2O + MA + NH_3 (purple trace) respectively (~45-50% RH). Each size distribution represents the average over five replicate measurements (± 1 standard deviation). Concentrations of the reactants are [MSA] = 6.2×10^{10} molecules per cm^3; [MA] = 0 or 6.0×10^{10} molecules per cm^3; [NH_3] = 0 or 2.8×10^{11} molecules per cm^3.

8. Determination of particle formation rates ($J_{>2.0nm}$) for the MSA + TMA + NH_3 reaction, dry conditions.

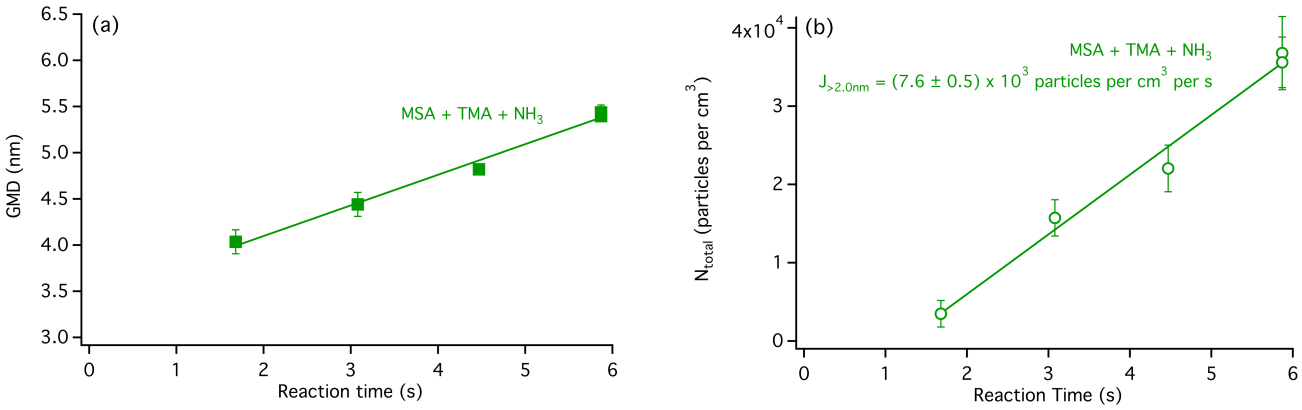

Figure S9. (a) Mobility geometric mean diameters (GMD, nm) determined from the size distributions as a function of reaction time for the MSA + TMA + NH_3 reaction. (b) Total number concentrations (N_{total}) measured using SMPS as a function of reaction time. Each data point corresponds to the average N_{total} measured from five successive scans ± 1 standard deviation. Concentrations of the reactants are [MSA] = 7.9×10^{10} molecules per cm^3; [TMA] = 5.0×10^{10} molecules per cm^3; [NH_3] = 2.2×10^{10} molecules per cm^3.

9. MSA + TMA (± NH_3), dry conditions – Variable reactant concentrations

9.1. Determination of $J_{>2.0nm}$ values from MSA + TMA (± NH_3) reaction under dry conditions a function of NH_3 concentration.

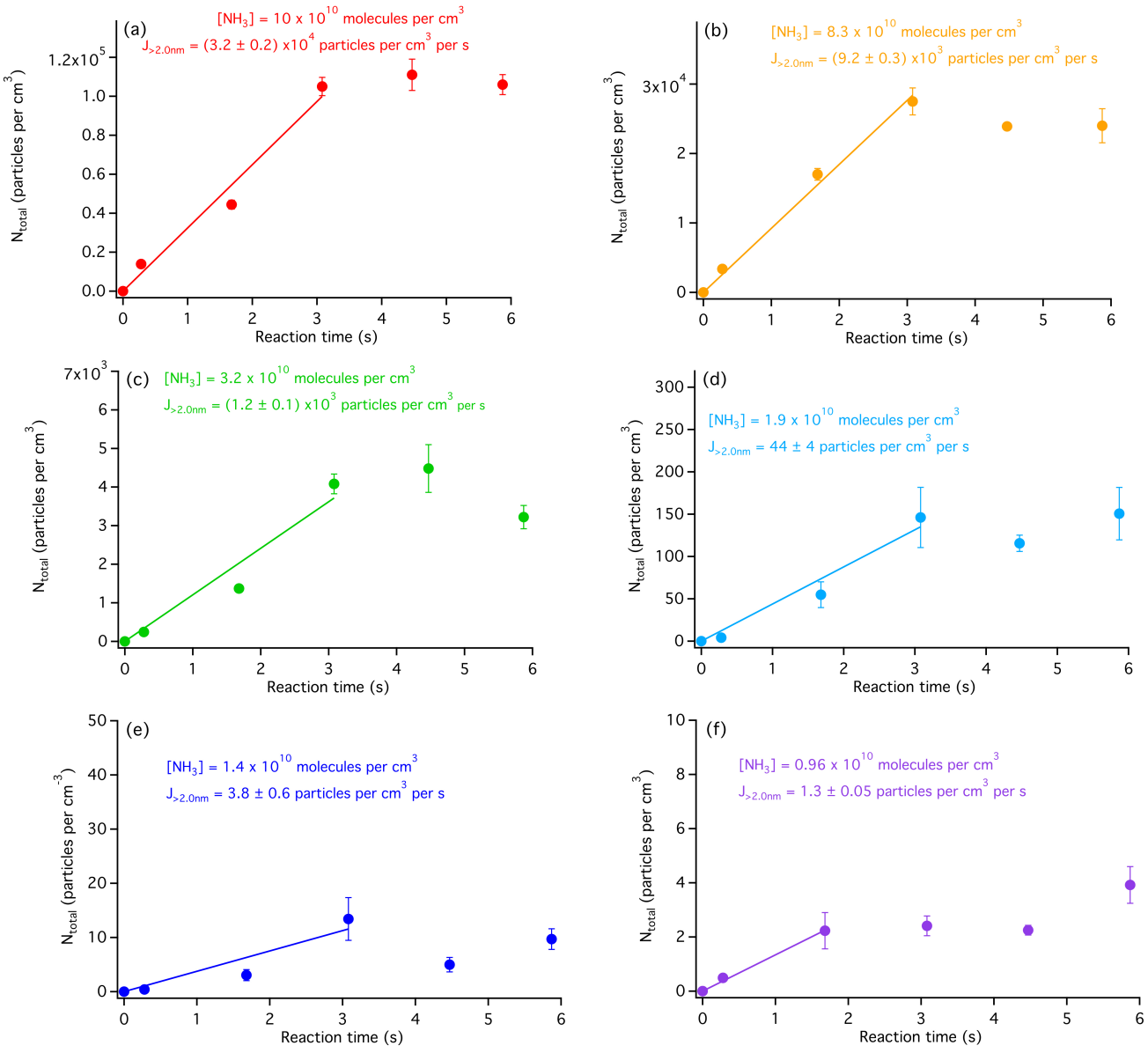

Figure S10. Determination of the particle formation rate ($J_{>2.0nm}$) using the CPC total number concentration (N_{total}) as a function of reaction time for the MSA + TMA + NH_3 system (same dataset as presented in Fig. 5). Each data point corresponds to the average N_{total} measured from three replicate CPC measurements ±1 standard deviation, each averaged over 2 min. Concentrations of the reactants are [MSA] = 6.4 × 10^{10} molecules per cm^3; [TMA] = (4.8) × 10^{10} molecules per cm^3; [NH_3] = 0.96 to 10 × 10^{10} molecules per cm^3.

9.2. MSA + TMA (± NH_3) (dry conditions) as a function of TMA concentration.

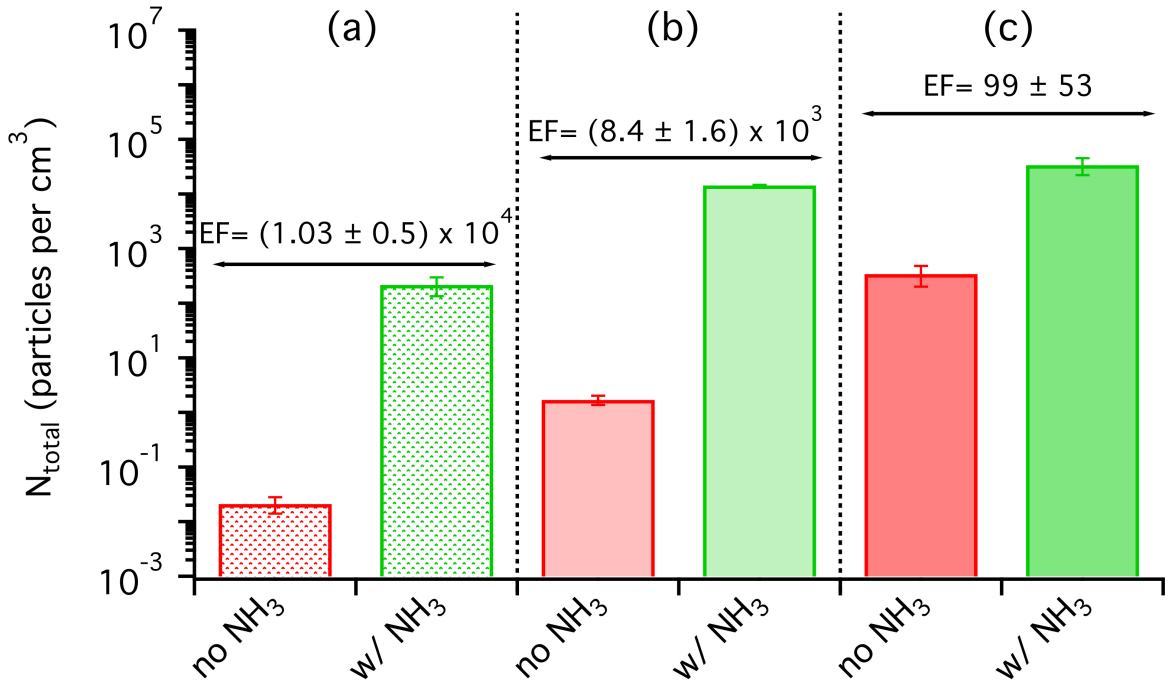

Figure S11. Total particle number concentrations (N_{total}) for the MSA + TMA reaction measured as a function of TMA concentration using the CPC with or without NH_3 at t = 5.3 s under dry conditions. Each data point corresponds to the average N_{total} measured from three replicate CPC measurements ±1 standard deviation, each averaged over 2 min. Concentrations of the reactants are [MSA] = 6.4×10^{10} molecules per cm^3 and [NH_3] = 0 or 1.8×10^{10} molecules per cm^3. TMA concentrations are (a) 1.4×10^{10} molecules per cm^3 ([MSA]/[TMA] = 5), (b) 3.0×10^{10} molecules per cm^3 ([MSA]/[TMA] ~ 2) and (c) 6.4×10^{10} molecules per cm^3 ([MSA]=[TMA]).

9.3. MSA + TMA (± NH_3) (~45-50% RH) as a function of TMA concentration.

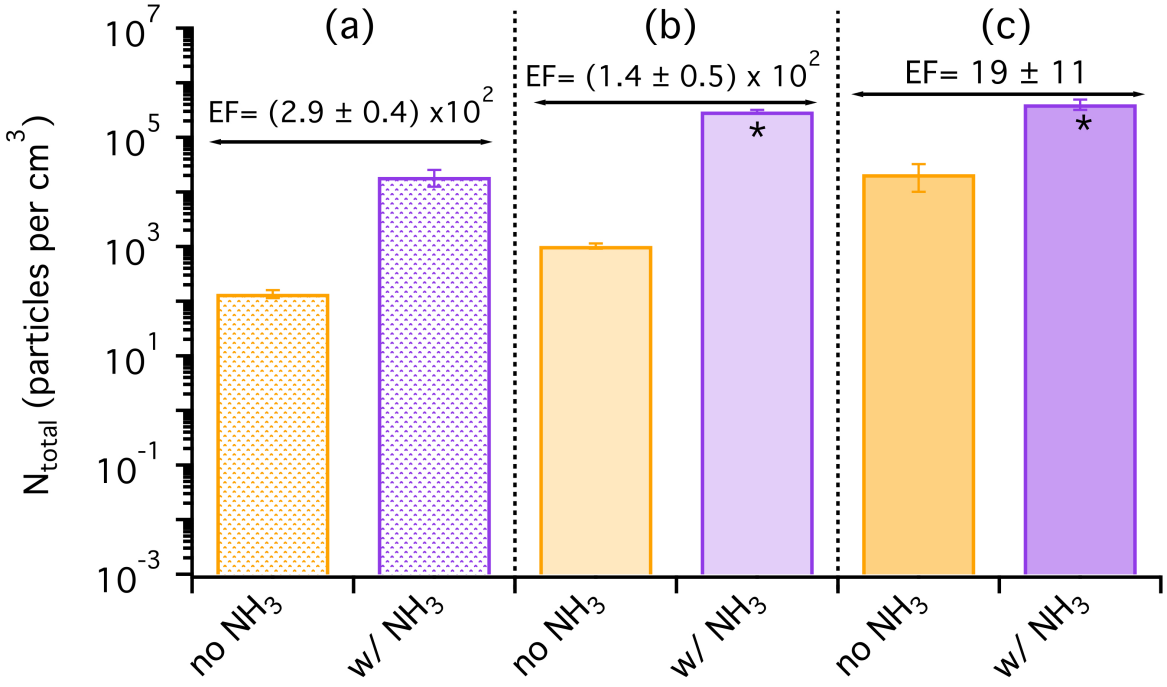

Figure S12. Total particle number concentrations (N_{total}) for the MSA + TMA reaction measured as a function of TMA concentration using the CPC with or without NH_3 at t = 5.3 s at ~45-50% RH. Each data point corresponds to the average N_{total} measured from three replicate CPC measurements ±1 standard deviation, each averaged over 2 min. Concentrations of the reactants are [MSA] = 6.4×10^{10} molecules per cm^3 and [NH_3] = 0 or 1.8×10^{10} molecules per cm^3. TMA concentrations are (a) 1.4×10^{10} molecules per cm^3 ([MSA]/[TMA] = 5), (b) 3.0×10^{10} molecules per cm^3 ([MSA]/[TMA] ~ 2) and (c) 6.4×10^{10} molecules per cm^3 ([MSA]=[TMA]). Note the data marked with an asterisk are lower limit values as the total concentration measured was higher than the CPC limit of 3×10^5 particles per cm^3.

10. Determination of particle formation rates ($J_{>2.0nm}$) for the MSA + TMA (± NH_3) reaction at high relative humidity (~45-50% RH).

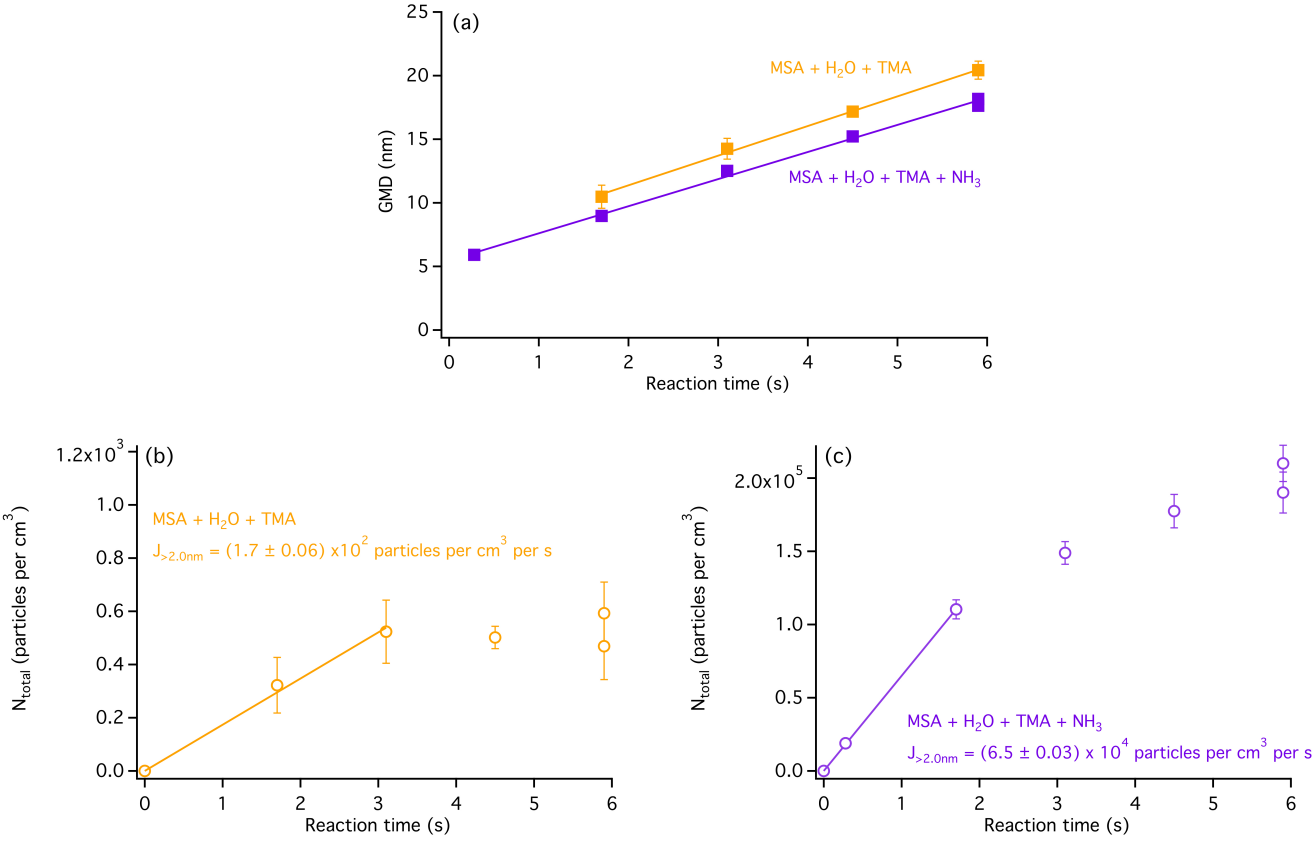

Figure S13. (a) Mobility geometric mean diameters (GMD, nm) determined from the size distributions as a function of reaction time for MSA + TMA + H_2O (orange trace) and MSA + TMA + H_2O + NH_3 (purple trace) respectively (~45-50% RH). Total number concentration (N_{total}) measured using the SMPS as a function of reaction time for (b) MSA + TMA + H_2O and (c) MSA + TMA + H_2O + NH_3 reactions. Each data point corresponds to the average N_{total} measured from five successive scans ± 1 standard deviation. Concentrations of the reactants are [MSA] = 7.9×10^{10} molecules per cm^3; [TMA] = 5.0×10^{10} molecules per cm^3; [NH_3] = 0 or 2.2×10^{10} molecules per cm^3.

11. Addition of TMA to MSA + NH_3 binary reaction system (dry conditions).

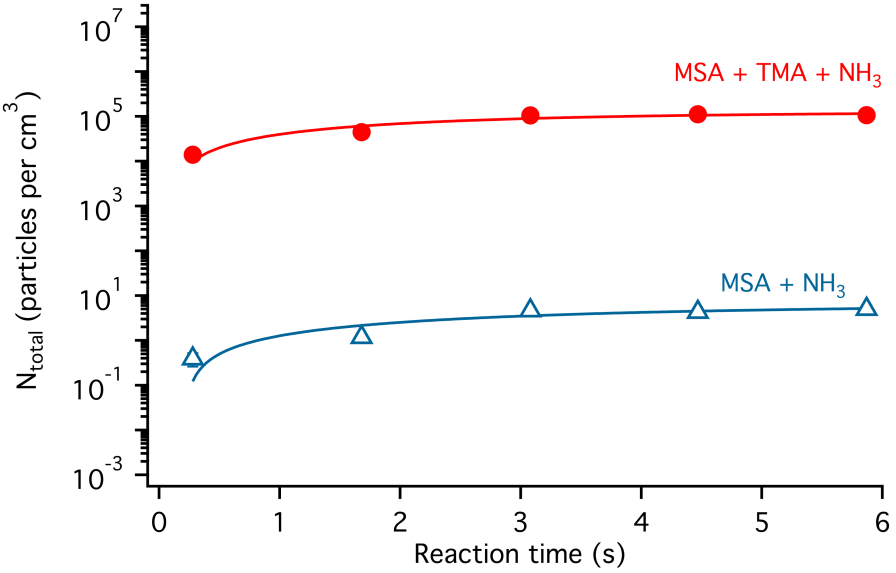

Figure S14. (a) Total particle concentration (N_{total}) measured using the CPC from the MSA + NH_3 and the MSA + NH_3 + TMA reactions as a function of reaction time. Each data point corresponds to the average N_{total} measured from three replicate CPC measurements ±1 standard deviation, each averaged over 2 min. Concentrations of reactants are [MSA] = 6.4×10^{10} molecules per cm^3; [TMA] = 0 or 4.0×10^{10} molecules per cm^3; [NH_3] = 1.0×10^{11} molecules per cm^3. At t = 5.9 s, the enhancement factor EF is $(2.1 \pm 0.5) \times 10^4$.

12. The cartesian coordinates and energies at B3LYP-D3/cc-pVDZ (in Hartree) of the lowest-energy isomer in each system.

1) MSA-MA E= -760.2770102

S	0.86707	0.14215	-0.00001
O	1.13672	1.60898	0.00000
O	0.12974	-0.35799	-1.25732
C	2.46246	-0.70902	0.00002
H	2.27601	-1.78705	-0.00001
H	2.99415	-0.39332	-0.90317
H	2.99410	-0.39335	0.90325
O	0.12972	-0.35799	1.25730
H	-1.42051	-0.68170	0.78935
N	-2.13712	-0.71146	-0.00001
H	-1.42056	-0.68171	-0.78938
H	-2.66054	-1.58501	0.00001
C	-3.00224	0.49369	0.00001
H	-3.62959	0.50257	0.89725
H	-2.34756	1.37085	-0.00006
H	-3.62971	0.50252	-0.89715

2) MSA-MA-H_2O E= -836.7485935

S	-1.12887	0.11411	-0.00348
O	-0.49734	0.64581	-1.28512
O	-1.17489	-1.40211	0.04438
C	-2.84368	0.67654	0.01037
H	-3.29933	0.31369	0.93691
H	-2.83004	1.76994	-0.02860
H	-3.33406	0.25031	-0.87040
O	-0.45847	0.71617	1.22939
H	1.28541	0.67287	0.75666
O	1.42129	-2.25448	0.08086
H	0.44540	-2.07025	0.09058
H	1.54266	-2.97464	-0.54736
N	1.94529	0.45497	-0.02729
H	1.33372	0.67977	-0.83952
H	2.03279	-0.58597	-0.03080
C	3.22854	1.18736	0.01422
H	3.03019	2.26392	0.02193
H	3.77726	0.91061	0.92037
H	3.82712	0.93267	-0.86669

3) 2MSA-2MA E=-1520.617083

S	-2.54761	0.00732	0.06667
O	-1.68312	-0.03387	-1.18300
O	-2.36877	1.31056	0.83529

C	-4.27515	-0.02740	-0.46543
H	-4.89281	0.04255	0.43584
H	-4.43477	0.82762	-1.12973
H	-4.43407	-0.97597	-0.98845
O	-2.36099	-1.22852	0.93501
H	-0.88505	-1.96340	0.46439
N	-0.02782	-2.15689	-0.11231
H	-0.08112	-1.48108	-0.88732
H	0.87279	-1.94442	0.39455
S	2.54881	-0.00350	0.06751
O	1.68667	0.01757	-1.18353
O	2.34080	-1.27592	0.87746
C	4.27485	-0.03172	-0.46581
H	4.42132	-0.95359	-1.03705
H	4.43794	0.85588	-1.08474
H	4.89802	-0.01525	0.43393
O	2.38311	1.26133	0.89626
H	0.87984	1.95339	0.46314
N	0.02780	2.16475	-0.11547
H	0.09172	1.52308	-0.91674
H	-0.88136	1.93831	0.37147
H	0.04087	3.13103	-0.43305
H	-0.03198	-3.10878	-0.47135

4) MSA-MA-NH_3 E=-816.8737778

S	-1.16136	-0.06972	-0.00218
O	-0.50334	-0.60288	-1.27354
O	-1.28043	1.43551	0.01744
C	-2.84426	-0.73084	0.01529
H	-3.32220	-0.37952	0.93519
H	-3.35385	-0.34580	-0.87370
H	-2.76761	-1.82210	-0.00673
O	-0.47254	-0.62932	1.24502
H	1.25486	-0.74404	0.75945
N	1.92318	-0.54429	-0.02032
H	1.30455	-0.74416	-0.83270
H	2.03053	0.51135	-0.01429
C	3.18697	-1.30414	0.01442
H	3.74153	-1.05219	0.92504
H	2.97142	-2.37793	0.00704
H	3.79467	-1.04991	-0.86102
N	1.60177	2.25026	0.00343
H	1.83919	2.82476	-0.80278
H	1.83131	2.79848	0.83004
H	0.57688	2.13800	-0.00201

5) MSA-MA-NH_3-H_2O E=-893.344011

S	-1.38363	0.06044	0.13937
O	-1.09817	-0.93012	-0.98065
O	-1.31043	1.50021	-0.30671
C	-3.09181	-0.24302	0.64782
H	-3.32607	0.47044	1.44401
H	-3.72368	-0.08342	-0.23151
H	-3.15106	-1.27647	1.00254
O	-0.53358	-0.22152	1.38055
H	1.08190	-0.14894	0.97802
N	2.02708	-0.10689	0.50855
H	2.06419	-0.95821	-0.08214
H	1.96329	0.71569	-0.15689
C	3.14406	0.01309	1.46640
H	3.01421	0.92603	2.05752
H	3.15107	-0.85177	2.13880
H	4.09611	0.06223	0.92624
N	1.43358	1.96780	-1.30970
H	1.48296	1.65688	-2.27830
H	1.75408	2.93313	-1.29339
H	0.43585	1.96786	-1.05467
O	1.33031	-2.01998	-1.35230
H	0.40185	-1.67943	-1.25975
H	1.25017	-2.97645	-1.42479

6) 2MSA-2MA-2NH_3 E=-1633.803473

S	2.68443	0.00028	-0.22083
O	2.36834	1.26867	-0.99598
O	2.36315	-1.26250	-1.00291
C	4.48350	-0.00365	-0.02134
H	4.75094	-0.90941	0.53155
H	4.92248	-0.00316	-1.02372
H	4.75452	0.89955	0.53401
O	2.09042	-0.00242	1.17398
H	0.00270	2.53988	0.61428
N	0.00301	2.54825	-0.44130
H	0.85936	2.01997	-0.72458
H	-0.85011	2.01457	-0.72402
C	-0.00328	3.91576	-1.00057
H	-0.90002	4.44461	-0.66027
H	0.89072	4.45174	-0.66428
H	-0.00566	3.86513	-2.09469
S	-2.68300	0.00042	-0.22077
O	-2.36229	-1.26453	-0.99953
O	-2.36034	1.26635	-0.99714
C	-4.48264	0.00161	-0.02705

H	-4.75276	0.90615	0.52654
H	-4.91874	0.00206	-1.03068
H	-4.75398	-0.90277	0.52621
O	-2.09416	-0.00141	1.17622
H	0.00079	-2.53832	0.61139
N	0.00078	-2.54662	-0.44417
H	-0.85313	-2.01414	-0.72691
H	0.85614	-2.01710	-0.72810
C	-0.00354	-3.91468	-1.00216
H	0.89104	-4.44913	-0.66494
H	-0.89963	-4.44439	-0.66148
H	-0.00564	-3.86535	-2.09634
N	-0.00125	1.92693	2.28287
H	-0.82162	1.32118	2.20874
H	-0.00198	2.36342	3.19976
H	0.81844	1.32010	2.21061
N	-0.00285	-1.93170	2.28176
H	0.81690	-1.32480	2.21125
H	-0.00358	-2.37094	3.19734
H	-0.82317	-1.32570	2.20941

7) 2MSA-2MA-2H_2O E=-1673.557936

S	2.64683	0.25054	-0.11420
O	2.32938	1.54825	-0.79058
O	1.97712	0.11999	1.22943
C	4.41583	0.29402	0.22062
H	4.68942	-0.63824	0.71878
H	4.93799	0.39405	-0.73299
H	4.61598	1.15137	0.86623
O	2.42298	-0.94484	-0.98747
H	0.71870	2.23670	-0.83664
O	-0.14969	1.81436	2.04359
H	0.67920	1.30002	1.93448
H	-0.86301	1.15327	1.90857
N	-0.19824	2.64594	-0.55718
H	-0.20723	2.55933	0.49192
H	-0.96672	2.01626	-0.87101
C	-0.37656	4.03690	-1.03620
H	0.43331	4.65736	-0.64695
H	-0.35793	4.05138	-2.12805
H	-1.33673	4.41736	-0.68152
S	-2.61911	-0.24045	-0.15996
O	-2.28850	-1.49026	-0.91507
O	-1.95921	-0.19047	1.19408
C	-4.38990	-0.31466	0.15955
H	-4.67155	0.58236	0.71466

H	-4.90569	-0.35565	-0.80189
H	-4.58988	-1.21279	0.74719
O	-2.39729	1.00992	-0.95333
H	1.00780	-1.97921	-0.98913
O	0.15455	-1.93313	1.92354
H	-0.67218	-1.41028	1.84028
H	0.87021	-1.26603	1.83903
N	0.23030	-2.61710	-0.71801
H	-0.67903	-2.18747	-0.99000
H	0.22358	-2.57915	0.33465
C	0.40435	-3.98649	-1.25687
H	0.40538	-3.95163	-2.34847
H	1.35416	-4.39227	-0.90253
H	-0.41820	-4.61584	-0.91080

8) 2MSA-2MA-2H_2O-2NH_3 E= -1786.733814

S	2.81616	-0.17724	-0.21566
O	2.89386	1.33499	-0.24001
O	1.85445	-0.71493	-1.26283
C	4.45928	-0.78136	-0.66928
H	4.43232	-1.87470	-0.63349
H	4.66926	-0.41902	-1.68007
H	5.16904	-0.37367	0.05698
O	2.53139	-0.73977	1.17018
H	0.04463	2.61872	0.04753
N	0.34421	2.29367	-0.92313
H	1.30483	1.91451	-0.81751
H	-0.30439	1.52827	-1.19867
C	0.28142	3.40313	-1.89788
H	-0.74771	3.77365	-1.94837
H	0.94862	4.20947	-1.57505
H	0.59121	3.04600	-2.88554
S	-2.73815	0.48807	-0.50197
O	-2.58506	-0.64965	0.50755
O	-1.63979	0.40822	-1.55901
C	-4.28976	0.15048	-1.36980
H	-4.42070	0.93218	-2.12434
H	-4.20621	-0.83921	-1.82921
H	-5.09025	0.17770	-0.62397
O	-2.87298	1.84616	0.12526
H	0.00194	-2.71192	0.42253
N	-0.35685	-2.10432	-0.36001
H	-1.13425	-1.52529	0.01476
H	0.42741	-1.47720	-0.63442
C	-0.82336	-2.86655	-1.53753
H	0.00099	-3.47007	-1.93150

H	-1.65181	-3.52012	-1.24376
H	-1.16093	-2.15626	-2.29868
N	-0.52815	2.91150	1.65693
H	-1.48493	2.57679	1.52506
H	-0.57171	3.81500	2.11961
H	-0.04013	2.26140	2.27702
N	0.71977	-3.22722	1.97835
H	1.60233	-2.71512	1.97182
H	0.87530	-4.12512	2.42706
H	0.06864	-2.68097	2.55400
O	-1.16307	-1.11094	2.96752
H	-0.47777	-0.42230	3.04337
H	-1.75455	-0.80977	2.25680
O	1.07023	0.65997	2.99040
H	1.60525	0.71138	3.78939
H	1.64733	0.22614	2.31702

9) MSA-TMA E=-838.9077982

S	1.43549	0.08537	-0.01891
O	1.73591	1.54220	-0.18471
O	0.94415	-0.62102	-1.26230
C	2.96252	-0.73407	0.50294
H	3.28161	-0.26792	1.44040
H	2.74372	-1.79813	0.63447
H	3.69679	-0.57118	-0.29261
O	0.44937	-0.17959	1.15808
H	-0.87715	-0.14021	0.56302
N	-1.87444	-0.04235	0.08255
C	-2.85636	0.20181	1.16471
H	-2.83543	-0.64282	1.86154
H	-2.57440	1.11551	1.69831
H	-3.86333	0.31115	0.74181
C	-1.76331	1.11724	-0.84641
H	-1.42722	1.98971	-0.27718
H	-1.00792	0.87900	-1.60059
H	-2.73883	1.31055	-1.31035
C	-2.13116	-1.30955	-0.64943
H	-1.29766	-1.46760	-1.33997
H	-2.16648	-2.13191	0.07304
H	-3.08609	-1.24090	-1.18651

10) MSA-TMA-H_2O E= -915.3751333

S	1.51187	-0.15080	-0.03995
O	1.56419	1.26171	-0.58413
O	1.18842	-1.20486	-1.06713
C	3.15521	-0.51616	0.61920

H	3.37038	0.21989	1.39977
H	3.13012	-1.53436	1.01960
H	3.85878	-0.43198	-0.21507
O	0.56072	-0.24021	1.16923
H	-0.85563	-0.26229	0.51330
N	-1.82072	-0.45800	0.07433
C	-1.95360	-1.93844	0.12689
H	-1.10690	-2.36680	-0.41876
H	-1.91424	-2.25793	1.17305
H	-2.90624	-2.23819	-0.32637
C	-2.82730	0.25193	0.90564
H	-2.76658	-0.12651	1.93156
H	-2.58093	1.31785	0.88699
H	-3.83041	0.07353	0.49887
C	-1.80824	0.03653	-1.33556
H	-1.67922	1.12148	-1.31967
H	-0.96286	-0.43109	-1.84827
H	-2.75810	-0.23523	-1.81296
O	-0.74246	2.67428	0.06266
H	0.12288	2.23846	-0.11383
H	-0.52933	3.60136	0.20863

11) 2MSA-2TMA E= -1677.856363

S	-3.11737	0.50285	-0.08791
O	-3.19793	-0.47574	-1.23415
O	-2.81738	1.92421	-0.46355
C	-4.74063	0.50409	0.71835
H	-4.96160	-0.52075	1.03248
H	-4.68408	1.18217	1.57544
H	-5.46591	0.85834	-0.02109
O	-2.14137	-0.01827	0.99652
H	-1.39166	-1.31124	0.46201
N	-0.92396	-2.20594	0.11359
C	0.08779	-2.60062	1.13499
H	0.80218	-1.78278	1.25597
H	-0.43546	-2.79729	2.07667
H	0.61613	-3.49656	0.79260
C	-2.01223	-3.20991	-0.02431
H	-2.46992	-3.36706	0.95803
H	-2.75709	-2.80811	-0.71651
H	-1.59240	-4.15229	-0.39529
C	-0.30281	-1.89243	-1.20673
H	-1.09206	-1.52327	-1.86632
H	0.46990	-1.13808	-1.06032
H	0.17294	-2.79473	-1.60412
S	3.11567	-0.50581	-0.08998

O	3.19880	0.47355	-1.23542
O	2.82535	-1.92886	-0.46601
C	4.73342	-0.49733	0.72727
H	4.94257	0.52793	1.04796
H	4.67731	-1.18034	1.58043
H	5.46669	-0.84119	-0.00914
O	2.12926	0.01106	0.98776
H	1.39130	1.30794	0.45500
N	0.92654	2.20748	0.11303
C	-0.08762	2.59400	1.13535
H	-0.79641	1.77104	1.25266
H	0.43383	2.79114	2.07787
H	-0.62211	3.48694	0.79494
C	2.01734	3.21013	-0.01337
H	2.47433	3.35662	0.97097
H	2.76232	2.81415	-0.70893
H	1.59993	4.15693	-0.37598
C	0.30882	1.90783	-1.21240
H	1.09806	1.53308	-1.86892
H	-0.47534	1.16349	-1.07404
H	-0.15239	2.81834	-1.60861

12) MSA-TMA-NH_3 E=-895.4972419

S	1.51079	-0.15447	-0.06721
O	1.69937	1.05633	-0.93949
O	1.11510	-1.41201	-0.80301
C	3.09474	-0.48080	0.74535
H	3.36492	0.41484	1.31317
H	2.96083	-1.34751	1.39995
H	3.82377	-0.68595	-0.04512
O	0.52897	0.12299	1.09823
H	-0.87633	-0.13063	0.47974
N	-1.82537	-0.44268	0.06737
C	-1.88028	-1.91357	0.28361
H	-1.01200	-2.35688	-0.21274
H	-1.82517	-2.11136	1.35923
H	-2.81855	-2.30875	-0.12490
C	-2.89180	0.28759	0.80052
H	-2.80730	0.05661	1.86783
H	-2.73249	1.35773	0.63506
H	-3.87407	-0.02819	0.42714
C	-1.81868	-0.09933	-1.38486
H	-1.73606	0.98706	-1.47153
H	-0.94812	-0.57927	-1.84075
H	-2.74984	-0.46018	-1.83919
N	-0.69818	2.73691	0.08457

H	-0.74820	3.75119	0.01496
H	0.08845	2.43260	-0.49579
H	-0.38899	2.51866	1.03123

13) 2MSA-2TMA-2NH_3 E= -1791.044745

S	2.13278	-1.93216	0.03194
O	3.21327	-1.00671	-0.44899
O	0.84520	-1.80313	-0.78904
C	2.71711	-3.62503	-0.23429
H	3.62244	-3.75236	0.36710
H	1.92620	-4.30895	0.08868
H	2.93084	-3.73348	-1.30195
O	1.82748	-1.82241	1.51928
N	-2.38179	-2.32544	-0.05963
H	0.20428	-1.21593	1.67036
C	-1.83490	-3.68454	-0.06149
H	-0.80918	-3.65063	-0.44544
H	-1.81870	-4.07820	0.96421
H	-2.43626	-4.37184	-0.68742
C	-3.73317	-2.28103	0.50886
H	-3.71585	-2.68611	1.53056
H	-4.07284	-1.24023	0.54370
H	-4.44954	-2.88001	-0.08603
C	-2.35995	-1.74324	-1.40946
H	-2.70480	-0.70585	-1.36501
H	-1.33417	-1.76867	-1.78997
H	-3.01124	-2.31185	-2.10083
N	-0.76995	-0.83887	1.67079
H	-0.76904	0.16445	1.37620
H	-1.16929	-0.89651	2.60423
H	-1.37979	-1.39972	0.98187
S	-2.12761	1.93077	-0.01859
O	-1.82579	1.82512	-1.50702
O	-0.84013	1.78983	0.80022
C	-2.70033	3.62662	0.25443
H	-3.60568	3.76211	-0.34518
H	-2.91170	3.73283	1.32276
H	-1.90540	4.30649	-0.06734
O	-3.21351	1.01057	0.46023
N	2.37470	2.33040	0.04279
H	0.75724	-0.17708	-1.35669
C	3.71852	2.28990	-0.54320
H	4.06418	1.25090	-0.57437
H	3.68529	2.68642	-1.56791
H	4.43938	2.89778	0.03703
C	1.81845	3.68552	0.04149

H	1.78463	4.07082	-0.98698
H	0.79843	3.64722	0.43993
H	2.42324	4.38224	0.65352
C	2.37285	1.75630	1.39615
H	1.35141	1.77643	1.78857
H	2.72383	0.72094	1.35295
H	3.02870	2.33296	2.07647
N	0.76247	0.82206	-1.66499
H	-0.20966	1.20437	-1.67181
H	1.16568	0.86367	-2.59759
H	1.37296	1.38978	-0.98230

14) MSA-TMA-NH_3-H_2O E= -971.9640828

S	1.53991	-0.47012	0.03951
O	2.20885	0.86054	-0.15975
O	0.99493	-1.10957	-1.21553
C	2.80087	-1.58396	0.70789
H	3.16387	-1.14613	1.64279
H	2.33135	-2.55781	0.87677
H	3.59945	-1.64960	-0.03799
O	0.44764	-0.42145	1.13639
H	-0.96861	-0.51044	0.41754
N	-1.90510	-0.65028	-0.08294
C	-1.93573	-2.08073	-0.49342
H	-1.05646	-2.27127	-1.11479
H	-1.89100	-2.70129	0.40755
H	-2.86379	-2.28237	-1.04163
C	-2.98484	-0.31273	0.88518
H	-2.88760	-0.96803	1.75718
H	-2.84918	0.72994	1.18680
H	-3.95986	-0.47015	0.40778
C	-1.90689	0.26364	-1.26175
H	-1.82238	1.28838	-0.89115
H	-1.03919	0.01438	-1.87850
H	-2.84087	0.12388	-1.81973
N	0.52014	3.25356	-0.78161
H	0.27177	3.34282	-1.76435
H	1.18280	2.47395	-0.70297
H	1.02594	4.10021	-0.53127
O	-1.02666	2.10165	1.31143
H	-0.59230	2.64593	0.61548
H	-0.35383	1.42928	1.50846

15) 2MSA-2TMA-$2H_2O$ E= -1830.780932

S	3.11232	0.80408	-0.14454
O	2.30458	1.71026	0.76368

O	2.47186	0.55322	-1.49245
C	4.67890	1.66028	-0.45192
H	5.16163	1.81983	0.51706
H	5.28504	1.02115	-1.10118
H	4.44083	2.61055	-0.93980
O	3.48967	-0.50514	0.54528
H	2.15202	-1.54849	0.25692
N	1.67542	-2.38645	-0.16637
C	2.60759	-2.83730	-1.23607
H	2.72342	-2.01022	-1.94222
H	3.57704	-3.06514	-0.78360
H	2.18981	-3.72321	-1.72778
C	1.52204	-3.38583	0.92391
H	2.51261	-3.62052	1.32671
H	0.90572	-2.93405	1.70422
H	1.05123	-4.28975	0.52025
C	0.35424	-1.97862	-0.73443
H	-0.28896	-1.63211	0.07310
H	0.52972	-1.18080	-1.45742
H	-0.10261	-2.84290	-1.22733
O	0.84666	-0.53026	2.04863
H	1.40006	0.25319	1.89407
H	0.01248	-0.20798	2.43695
S	-3.22232	-0.68783	-0.39401
O	-2.62273	-1.33589	0.84687
O	-2.43519	-0.95251	-1.64599
C	-4.85474	-1.43842	-0.61136
H	-5.43812	-1.23009	0.29057
H	-5.30921	-0.98292	-1.49661
H	-4.70273	-2.51325	-0.75034
O	-3.51250	0.79960	-0.15963
H	-2.23348	1.78285	-0.05808
N	-1.36676	2.37084	-0.23026
C	-1.75890	3.41960	-1.20526
H	-2.12248	2.93008	-2.11383
H	-2.55740	4.03105	-0.77240
H	-0.88662	4.04246	-1.43393
C	-0.87756	2.93910	1.05915
H	-1.57755	3.71178	1.39389
H	-0.84446	2.13242	1.79491
H	0.12481	3.35254	0.90793
C	-0.36729	1.43023	-0.82314
H	-0.04558	0.73845	-0.04499
H	-0.85408	0.88368	-1.63370
H	0.50371	1.98604	-1.16946
O	-1.73555	0.28038	2.80028

H	-2.15774	-0.29414	2.11262
H	-2.12999	0.01741	3.63800

16) 2MSA-2MA-2NH_3-2H_2O E= -1943.980514

S	2.70132	-1.31950	0.38495
O	3.67058	-0.26792	-0.11236
O	1.57251	-1.58445	-0.60563
C	3.63791	-2.86254	0.50358
H	4.45160	-2.69187	1.21488
H	2.95381	-3.63808	0.86166
H	4.02186	-3.09482	-0.49429
O	2.16315	-1.03989	1.77527
N	-1.47294	-2.77916	-0.56477
H	0.33918	-1.03154	1.67463
C	-0.68478	-3.98255	-0.29094
H	0.37465	-3.76256	-0.46375
H	-0.82023	-4.27988	0.75801
H	-0.98943	-4.83291	-0.93171
C	-2.89597	-2.99083	-0.27193
H	-3.02133	-3.24554	0.78774
H	-3.44888	-2.06610	-0.46657
H	-3.32124	-3.80634	-0.88807
C	-1.28276	-2.32141	-1.94699
H	-1.81367	-1.37439	-2.09531
H	-0.21435	-2.16808	-2.13196
H	-1.66471	-3.06393	-2.67440
N	-0.65853	-0.94595	1.41275
H	-0.87212	0.02461	1.11042
H	-1.31019	-1.13927	2.18199
H	-0.89412	-1.61591	0.61217
S	-2.70230	1.32110	-0.38707
O	-2.16323	1.03743	-1.77629
O	-1.57383	1.58674	0.60382
C	-3.63580	2.86574	-0.50957
H	-4.44827	2.69591	-1.22245
H	-4.02139	3.09980	0.48726
H	-2.94943	3.63962	-0.86692
O	-3.67390	0.27223	0.11126
N	1.47735	2.78044	0.56804
H	0.87163	-0.02121	-1.11035
C	2.90136	2.99297	0.28046
H	3.45369	2.06741	0.47264
H	3.02974	3.25233	-0.77774
H	3.32487	3.80591	0.90126
C	0.69060	3.98557	0.29782
H	0.82984	4.28853	-0.74898

H	-0.36950	3.76490	0.46574
H	0.99298	4.83247	0.94430
C	1.28265	2.31677	1.94768
H	0.21359	2.16297	2.12844
H	1.81279	1.36906	2.09394
H	1.66208	3.05614	2.67957
N	0.65740	0.94891	-1.41354
H	-0.34077	1.03373	-1.67415
H	1.30800	1.14077	-2.18410
H	0.89466	1.61925	-0.61439
O	3.25875	1.06989	-2.49593
H	3.48000	0.55500	-1.68600
H	3.73737	0.63851	-3.21105
O	-3.26399	-1.07450	2.48956
H	-3.74542	-0.64646	3.20479
H	-3.48435	-0.55742	1.68078

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