



*Supplement of*

## **Methane sulfonic acid enhanced formation of molecular clusters of sulfuric acid and dimethyl amine**

**N. Bork et al.**

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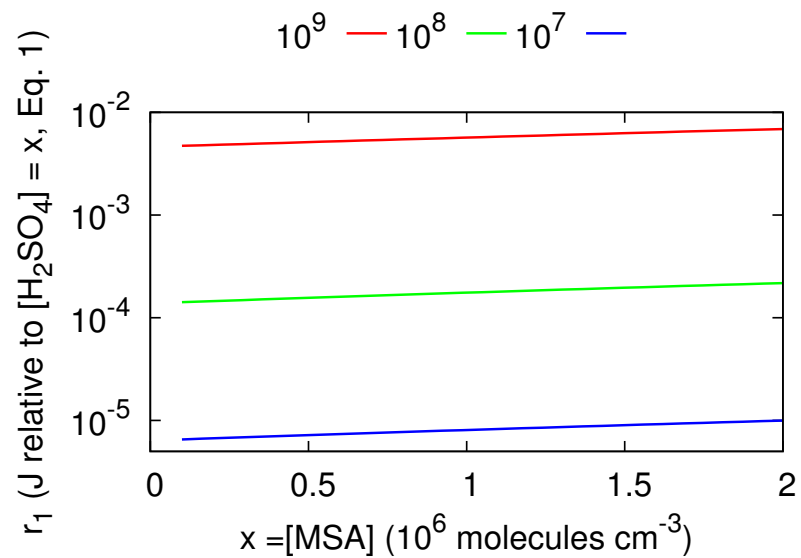


Figure S1: Ratio of MSA-DMA and  $\text{H}_2\text{SO}_4$ -DMA based cluster formation rates as defined in Equation 1 in the main article at the indicated DMA concentrations.

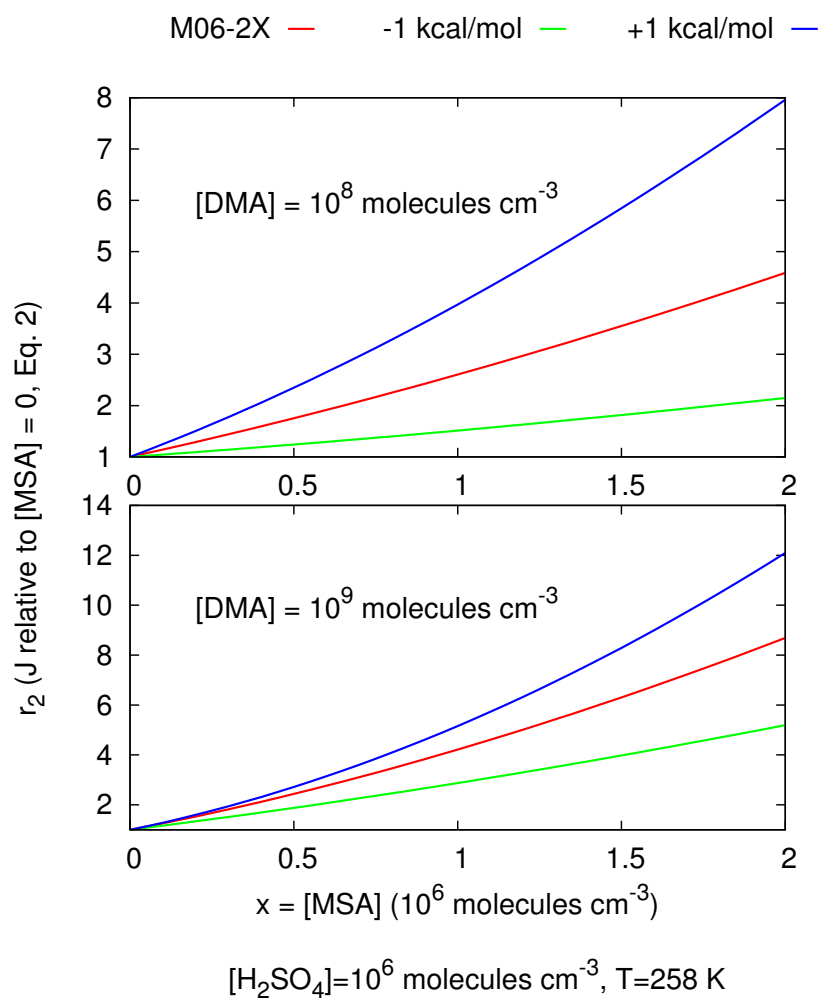


Figure S2: Enhancement factor as defined in Equation 2 in the main article assuming that all clusters are predicted too weakly bound (blue line) or too strongly bound (green line) by 1 kcal/mol, compared to the values presented in the main article (red line) using M06-2X/6-311++G(3df,3pd).

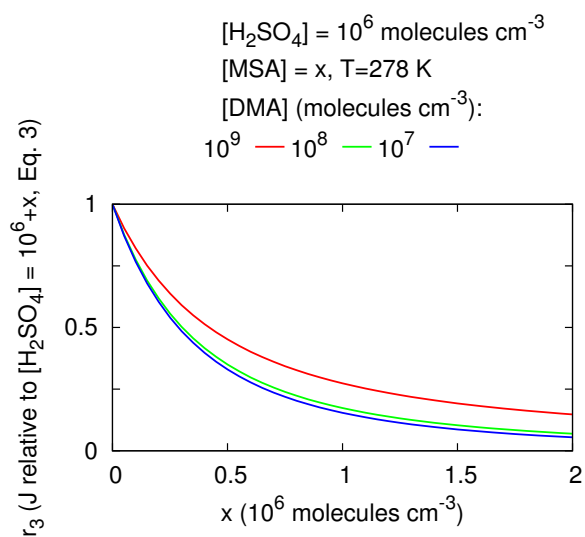


Figure S3: Cluster formation rate of added MSA relative to the same amount of added  $\text{H}_2\text{SO}_4$  as defined in Equation 3 for  $T=278 \text{ K}$ .

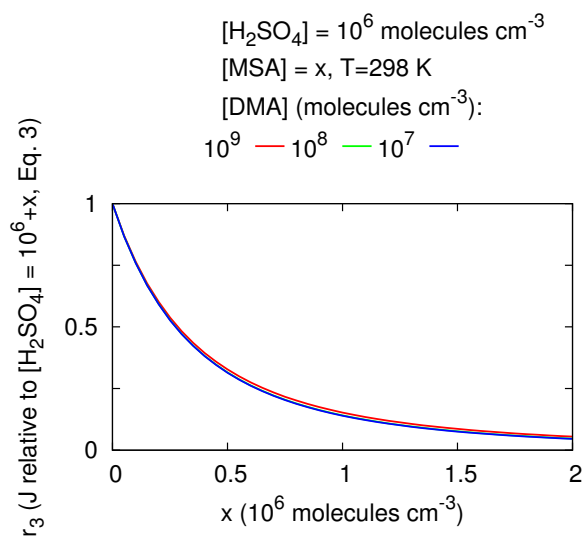


Figure S4: Cluster formation rate of added MSA relative the same amount of added  $\text{H}_2\text{SO}_4$  as defined in Equation 3 for  $T=298 \text{ K}$ .

Table S1: Energy differences between the investigated clusters and corresponding monomers calculated by M06-2X/6-311++G(3df,3pd). SA, MSA and DMA is shorthand for sulfuric acid, methane sulfonic acid and dimethyl amine, respectively. Units are kcal/mol and cal/(mol K).

Species	Binding enthalpy	Binding entropy	Binding Gibbs free energy (298.15 K)
<b>Dimers</b>			
(SA)(DMA)	-21.3705	-33.9220	-11.2575
(MSA)(DMA)	-18.6747	-37.7460	-7.4209
(SA) <sub>2</sub>	-18.4419	-33.7590	-8.3779
(MSA) <sub>2</sub>	-20.2799	-37.6040	-9.0688
(SA)(MSA)	-22.8577	-40.7860	-10.6978
(DMA) <sub>2</sub>	-3.8165	-27.7800	4.4660
<b>Trimers</b>			
(SA) <sub>2</sub> (DMA)	-53.2260	-77.3450	-30.1663
(SA)(MSA)(DMA)	-53.7889	-83.3270	-28.9458
(MSA) <sub>2</sub> (DMA)	-46.1602	-74.2440	-24.0248
(SA)(DMA) <sub>2</sub>	-36.0523	-73.5250	-14.1309
(MSA)(DMA) <sub>2</sub>	-23.6697	-66.9830	-3.6985
(SA) <sub>3</sub>	-36.8141	-76.7170	-13.9426
(MSA) <sub>3</sub>	-32.5652	-70.8040	-11.4558
(SA) <sub>2</sub> (MSA)	-38.4726	-75.6890	-15.9080
(SA)(MSA) <sub>2</sub>	-39.5557	-77.0310	-16.5901
<b>Tetramers</b>			
(SA) <sub>2</sub> (DMA) <sub>2</sub>	-78.8692	-118.3660	-43.5793
(SA)(MSA)(DMA) <sub>2</sub>	-74.9271	-117.9480	-39.7609
(MSA) <sub>2</sub> (DMA) <sub>2</sub>	-68.8152	-107.9090	-36.6428
(SA) <sub>3</sub> (DMA)	-77.4635	-118.7160	-42.0701
(SA) <sub>2</sub> (MSA)(DMA)	-78.1400	-120.3240	-42.2672
(SA)(MSA) <sub>2</sub> (DMA)	-73.3132	-119.8910	-37.5684
(MSA) <sub>3</sub> (DMA)	-67.7880	-119.7310	-32.0908
<b>Pentamers</b>			
(MSA) <sub>3</sub> (DMA) <sub>2</sub>	-91.6823	-155.3190	-45.3746
(SA)(MSA) <sub>2</sub> (DMA) <sub>2</sub>	-99.8123	-152.6910	-54.2884
(SA) <sub>2</sub> (MSA)(DMA) <sub>2</sub>	-102.2301	-156.8580	-55.4637
(SA) <sub>3</sub> (DMA) <sub>2</sub>	-106.4024	-155.6450	-59.9987
<b>Hexamer</b>			
(MSA) <sub>1</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub> (DMA) <sub>2</sub>	-128.8001	-197.3050	-69.9742

Table S2: Geometry of SA. Units are Å.

Atom	X	Y	Z
S	0.000063	0.000213	-0.15381100
O	-0.640599	1.069478	-0.81843000
O	0.641011	-1.067331	-0.82092200
O	1.029406	0.661681	0.83706000
H	1.691454	0.00903	1.10050100
O	-1.029838	-0.663878	0.83493300
H	-1.692302	-0.012025	1.099357

Table S3: Geometry of MSA. Units are Å.

Atom	X	Y	Z
S	-0.087635	0.134824	0.06611100
C	1.59981	-0.361314	-0.02558000
H	1.694967	-1.357427	0.39413100
H	1.905034	-0.334378	-1.06683400
H	2.16456	0.359484	0.55901300
O	-0.224539	1.393873	-0.57366500
O	-0.577492	-0.084946	1.38880100
O	-0.781313	-0.947124	-0.87364600
H	-1.294506	-1.551402	-0.322523

Table S4: Geometry of DMA. Units are Å.

Atom	X	Y	Z
N	-0.000005	0.568593	-0.14905600
H	-0.000009	1.334936	0.51053900
C	1.204279	-0.224049	0.02025200
H	1.261356	-0.962291	-0.78040300
H	1.240369	-0.765162	0.97608800
H	2.082759	0.414214	-0.05075900
C	-1.204267	-0.224048	0.02024800
H	-1.261392	-0.962248	-0.78044400
H	-2.082768	0.414205	-0.05068000
H	-1.240349	-0.765221	0.976058

Table S5: Geometry of DMA SA. Units are Å.

Atom	X	Y	Z
S	-1.267211	-0.174405	0.04944800
O	-0.553074	0.015717	1.29327800
O	-2.472918	-0.935944	0.07942600
O	-1.690617	1.324447	-0.34847000
H	-2.476306	1.272002	-0.90388100
O	-0.334249	-0.587655	-1.01995400
H	1.040231	-0.403877	-0.47126800
N	1.890413	-0.111827	0.15026500
H	1.502209	-0.288162	1.08064000
C	2.055402	1.346068	-0.01703900
H	2.344576	1.545194	-1.04539500
H	2.820147	1.713356	0.66296500
H	1.098925	1.815548	0.19674500
C	3.100559	-0.901202	-0.11983300
H	3.402389	-0.73476	-1.15034600
H	2.879331	-1.953878	0.02680000
H	3.902092	-0.593866	0.54771000

Table S6: Geometry of DMA MSA. Units are Å.

Atom	X	Y	Z
S	-1.100618	0.078767	-0.04975300
C	-2.653272	-0.748458	0.12148000
H	-3.245498	-0.51027	-0.75698400
H	-2.469712	-1.81597	0.18740900
H	-3.134518	-0.378092	1.02123300
O	-1.363539	1.493065	-0.11415000
O	-0.432522	-0.480243	-1.21373700
O	-0.351214	-0.297244	1.19148000
H	1.014493	-0.191819	0.89985500
N	2.077886	-0.031165	0.54885200
H	2.670933	0.04824	1.36975500
C	2.083583	1.245189	-0.20262300
H	1.444817	1.115424	-1.07206400
H	3.098831	1.495151	-0.50236700
H	1.661827	2.023189	0.42735000
C	2.48538	-1.189292	-0.27310100
H	1.741561	-1.299066	-1.05768400
H	2.492374	-2.079316	0.34941000
H	3.473637	-1.018845	-0.695115



Table S7: Geometry of SA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
S	-2.035878	-0.073295	0.11410000
O	-1.067705	0.085136	1.15676200
O	-3.310894	-0.604497	0.39602300
O	-2.182452	1.369579	-0.49135800
H	-2.960685	1.414409	-1.06354000
O	-1.423183	-0.88934	-1.03860300
H	-0.461344	-0.657678	-1.15613600
O	1.067511	-0.085828	-1.15658000
S	2.035801	0.073261	-0.11412700
O	1.42284	0.889095	1.03856700
O	3.310397	0.605324	-0.39632300
O	2.183503	-1.36941	0.49156900
H	0.46111	0.657026	1.15624300
H	2.962028	-1.413694	1.063402

Table S8: Geometry of MSA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
S	-1.837512	0.088864	0.04630000
O	-1.631683	1.490825	-0.12774400
O	-1.171603	-0.530195	1.17160800
O	-1.471288	-0.689158	-1.24427400
S	2.011557	-0.120252	-0.06790600
O	1.477945	-0.596611	1.31252200
H	0.484965	-0.612643	1.32817800
O	1.119985	-0.60661	-1.09926100
O	3.38258	-0.469435	-0.14712500
H	-0.472445	-0.723646	-1.31458100
C	-3.550707	-0.269048	0.14202500
H	-3.672895	-1.343574	0.22948000
H	-3.921904	0.24191	1.02576400
H	-4.02311	0.116639	-0.75591000
C	1.839751	1.628769	0.00431200
H	2.44072	1.98612	0.83455000
H	2.211322	2.018194	-0.93957200
H	0.786865	1.870352	0.133941

Table S9: Geometry of SA MSA. Units are Å.

Atom	X	Y	Z
S	-1.725635	0.001889	-0.06574300
C	-3.470936	0.002544	-0.18999500
O	-1.196641	-1.204753	-0.64397200
O	-1.200268	1.237458	-0.58241100
O	-1.563526	-0.037073	1.47832300
S	1.930346	-0.001246	0.08937900
O	1.5547	1.236764	-0.77108300
H	0.584065	1.388218	-0.76120900
O	1.06546	-0.020837	1.23930600
O	3.325213	-0.001707	0.25726700
O	1.559525	-1.212847	-0.80988100
H	0.588231	-1.360162	-0.81455900
H	-0.589652	-0.038628	1.66696000
H	-3.842552	-0.908648	0.26786000
H	-3.700831	0.029374	-1.25140900
H	-3.844727	0.888249	0.313766

Table S10: Geometry of DMA SA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
S	2.231577	0.028976	0.02757100
O	1.318603	1.06914	-0.38957900
O	3.59381	0.349805	0.18880300
O	1.696466	-0.563379	1.35199500
H	0.693365	-0.629809	1.32677100
O	2.127857	-1.136989	-0.98057900
H	1.186944	-1.45851	-1.04312100
S	-1.416599	-1.244316	-0.10513900
O	-0.878388	-0.615331	1.10468700
O	-0.386891	-1.915618	-0.87182900
O	-2.410617	-2.375884	0.37282200
H	-1.906976	-3.145181	0.66658800
O	-2.264284	-0.343175	-0.84641300
H	-1.768465	1.270039	-0.41880200
N	-1.180882	2.052867	-0.06939600
H	-0.240759	1.621913	0.02507600
C	-1.673905	2.497327	1.25004700
H	-2.663744	2.929444	1.13164600
H	-0.989994	3.241104	1.64951700
H	-1.714646	1.631303	1.90273600
C	-1.086714	3.124486	-1.08103700
H	-2.072059	3.551852	-1.24455500
H	-0.703138	2.696143	-2.00163900
H	-0.402733	3.887646	-0.720668

Table S11: Geometry of DMA MSA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
S	2.303408	-0.283323	-0.09729600
C	2.207511	-0.964188	1.52249100
H	1.157055	-1.044764	1.78901800
H	2.69331	-1.934869	1.49944400
H	2.7403	-0.285426	2.18245200
O	3.665634	-0.242987	-0.50525400
O	1.574005	0.971625	-0.08667200
O	1.551039	-1.296749	-0.97003900
H	0.528271	-1.124033	-1.04174000
S	-1.774458	-0.905025	-0.02497200
C	-2.596528	-2.465886	-0.04923500
H	-3.14411	-2.543316	-0.98318800
H	-1.841883	-3.243023	0.02525900
H	-3.270856	-2.498116	0.80095600
O	-0.895	-0.881032	-1.21425400
O	-1.005833	-0.821864	1.20289500
O	-2.808946	0.1177	-0.13595300
H	-1.743793	1.539129	-0.23845500
N	-0.871976	2.07249	-0.05341500
H	-0.085626	1.400711	-0.16035600
C	-0.870775	2.50385	1.36034600
H	-1.655347	3.240296	1.51093800
H	0.101582	2.932105	1.58795300
H	-1.04893	1.623316	1.97128600
C	-0.670588	3.161871	-1.02660800
H	-1.451488	3.906792	-0.90114100
H	-0.7084	2.744128	-2.02784800
H	0.305652	3.605795	-0.852127

Table S12: Geometry of DMA SA MSA. Units are Å.

Atom	X	Y	Z
S	2.326966	0.035878	-0.07242900
O	3.73458	0.064753	-0.15192200
O	1.591831	1.27003	-0.16700400
O	1.78841	-0.919672	-1.16951000
H	0.793895	-0.822561	-1.23928200
O	1.937554	-0.666581	1.25148300
H	0.95635	-0.870321	1.28064100
S	-1.51439	-1.083408	0.07352100
C	-1.969655	-2.731984	-0.35017400
H	-1.062302	-3.288409	-0.56599200
H	-2.489402	-3.157795	0.50273600
H	-2.618501	-2.689565	-1.21931300
O	-0.617369	-1.177922	1.22385100
O	-2.716969	-0.327277	0.32806800
O	-0.789004	-0.542597	-1.10628500
H	-0.762425	1.169544	-0.56391600
N	-0.919232	2.140137	-0.22517400
H	-0.084481	2.639057	-0.53315200
C	-0.956025	2.143364	1.26112100
H	-1.800702	1.538155	1.57408600
H	-1.064785	3.170439	1.59916800
H	-0.026218	1.715341	1.62050000
C	-2.156775	2.662175	-0.84438700
H	-2.969618	2.007779	-0.54260700
H	-2.046739	2.643109	-1.92406800
H	-2.3292	3.677529	-0.498847

Table S13: Geometry of DMA<sub>2</sub>SA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
N	-2.777147	-0.578147	0.06846700
H	-2.11094	0.173922	-0.21958900
C	-3.109701	-0.448095	1.50233100
H	-3.871639	-1.181206	1.75420000
H	-3.4716	0.558212	1.69247800
H	-2.208253	-0.634585	2.07703700
C	-3.94475	-0.509746	-0.83204300
H	-4.620043	-1.330528	-0.60774800
H	-3.59614	-0.581689	-1.85762800
H	-4.448812	0.441208	-0.68309100
S	-0.277839	2.096862	-0.17547300
O	1.158498	1.87648	-0.28002500
O	-0.720684	3.440873	-0.27685100
O	-0.997494	1.152325	-1.06886600
H	-0.067414	-0.167343	-1.38556300
O	-0.68917	1.615957	1.28229700
H	-0.353709	0.69595	1.36796200
S	0.258751	-1.86063	-0.10688000
O	0.497598	-0.988746	-1.40449000
O	0.129135	-0.895567	0.99203500
O	-0.972285	-2.604374	-0.30326000
H	-2.242127	-1.463351	-0.08338200
O	1.461348	-2.648273	-0.01189700
H	2.604809	-1.12515	-0.03788500
N	2.87478	-0.138727	0.10021900
H	2.025377	0.445532	-0.07815500
C	3.896047	0.273876	-0.88137400
H	4.812195	-0.284768	-0.71058300
H	4.0734	1.33909	-0.76245500
H	3.512143	0.075981	-1.87743000
C	3.260892	0.070819	1.50996400
H	4.175497	-0.476733	1.72073600
H	2.449239	-0.291891	2.13339100
H	3.409485	1.135235	1.669736

Table S14: Geometry of DMA<sub>2</sub>MSA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
H	-0.607653	-1.398838	0.26380200
S	2.64552	-0.042384	-0.23190100
O	2.426412	-1.3637	-0.82519800
O	2.641277	1.050373	-1.17787400
O	1.707447	0.186176	0.88271200
N	0.03016	-2.209236	0.12834700
H	0.905005	-1.85775	-0.32599200
C	-0.608081	-3.227103	-0.72799300
H	-1.527511	-3.56186	-0.25626100
H	0.082255	-4.057607	-0.85308100
H	-0.849959	-2.775906	-1.68349100
C	0.391941	-2.696652	1.47314500
H	-0.509842	-3.021892	1.98533900
H	0.857148	-1.874577	2.00815700
H	1.089304	-3.524542	1.37435600
H	0.607891	1.398971	0.26390400
S	-2.645497	0.042304	-0.23196200
O	-1.707521	-0.186117	0.88275500
O	-2.426115	1.363407	-0.82562700
O	-2.641417	-1.050711	-1.17762800
N	-0.030058	2.209222	0.12811900
H	-0.904753	1.857446	-0.32627500
C	0.608106	3.22696	-0.72843200
H	1.527388	3.562068	-0.25665700
H	-0.082381	4.057283	-0.85388100
H	0.850222	2.775525	-1.68375900
C	-0.392195	2.696999	1.47268700
H	0.509407	3.022673	1.98492500
H	-0.857279	1.874986	2.00790200
H	-1.089769	3.524661	1.37349200
C	4.261028	-0.103672	0.48822800
H	4.973116	-0.286229	-0.31081500
H	4.454277	0.853211	0.96331300
H	4.283929	-0.90878	1.21605700
C	-4.26101	0.104094	0.48808500
H	-4.973022	0.286594	-0.31104100
H	-4.454475	-0.852625	0.96340800
H	-4.283775	0.909391	1.215706



Table S15: Geometry of DMA<sub>2</sub>SA MSA. Units are Å.

Atom	X	Y	Z
N	-2.47052	-0.965765	0.39995100
H	-1.85682	-1.51988	-0.23315600
C	-3.68966	-0.526641	-0.30012500
H	-4.285878	0.078508	0.37783900
H	-4.255568	-1.398083	-0.61904200
H	-3.387465	0.067501	-1.15712800
C	-2.710381	-1.772746	1.61080300
H	-3.278007	-1.180899	2.32410200
H	-1.742527	-2.040158	2.02320400
H	-3.264865	-2.667117	1.33939300
S	-0.661743	1.926962	-0.09000600
O	0.774789	1.981654	0.16306300
O	-1.000415	1.090902	-1.25154400
H	0.174085	-0.029601	-1.58879800
O	-1.466617	1.57216	1.07081500
S	0.575719	-1.794631	-0.46481400
O	0.893432	-0.713386	-1.58626800
O	0.282609	-1.029942	0.74500000
O	-0.590646	-2.539304	-0.91149300
H	-1.924244	-0.125087	0.66606400
O	1.817474	-2.526023	-0.38108200
H	2.706415	-0.836507	0.16024900
N	2.770324	0.154296	0.43903800
H	1.833975	0.572375	0.26031100
C	3.749615	0.866038	-0.40118900
H	4.745033	0.471573	-0.21515300
H	3.707399	1.923288	-0.15523800
H	3.471405	0.716626	-1.44002000
C	3.011029	0.249413	1.89146300
H	3.980817	-0.180324	2.12760100
H	2.214583	-0.294427	2.38974800
H	2.979961	1.297869	2.17465600
C	-1.124885	3.575535	-0.53064200
H	-0.896345	4.222599	0.31076600
H	-0.554084	3.864124	-1.40780900
H	-2.189432	3.582533	-0.743201

Table S16: Geometry of DMA<sub>2</sub>SA<sub>3</sub>. Units are Å.

Atom	X	Y	Z
S	-3.820794	-0.614876	-0.49062900
O	-5.119344	-0.478945	-1.02136300
O	-3.337108	0.355554	0.45668800
O	-3.704431	-2.016768	0.14977300
H	-2.801157	-2.119583	0.55027700
O	-2.818651	-0.654698	-1.67801900
H	-1.880093	-0.606296	-1.34646200
N	3.743456	-1.49119	-0.15913500
H	3.394317	-0.679534	0.40077200
C	4.824819	-1.039116	-1.06309400
H	5.134563	-1.872844	-1.68728800
H	5.65845	-0.696594	-0.45687900
H	4.453127	-0.217007	-1.66648000
C	4.121245	-2.602119	0.73975300
H	4.446017	-3.448596	0.14095200
H	3.250648	-2.87158	1.32839800
H	4.932884	-2.270363	1.38082400
S	2.404369	1.54007	-0.32183100
O	1.290391	2.457293	-0.19709700
O	3.653564	2.073516	-0.74688300
O	2.526232	0.707198	0.90385300
H	1.133572	0.13915	1.49783000
O	2.012522	0.502335	-1.46222800
H	1.096524	0.171436	-1.31136800
S	-0.073186	-1.288943	0.52382100
O	0.237117	-0.273177	1.68010800
O	-0.40681	-0.435161	-0.64584700
O	1.128749	-2.048148	0.28388600
H	2.901031	-1.755296	-0.67853300
O	-1.208254	-2.04313	0.98249300
H	-1.678825	1.18118	0.55517200
N	-1.270675	2.120445	0.62502000
H	-0.257903	2.061089	0.40572800
C	-1.468876	2.614233	2.00170500
H	-2.535441	2.648274	2.20556600
H	-1.031907	3.60522	2.08725700
H	-0.981862	1.925869	2.68525700
C	-1.907183	2.959974	-0.41152300
H	-2.974556	3.003463	-0.21740000
H	-1.725762	2.502437	-1.37970500
H	-1.461156	3.949999	-0.380852

Table S17: Geometry of DMA<sub>2</sub>MSA<sub>3</sub>. Units are Å.

Atom	X	Y	Z
S	3.833352	-0.637394	-0.00336900
C	5.55806	-0.976843	0.01836500
H	5.706442	-1.784056	0.72959800
H	5.85987	-1.276962	-0.97978400
H	6.078449	-0.079724	0.33787200
O	3.417116	-0.173021	1.28940700
O	3.133895	-1.780334	-0.52741500
O	3.796567	0.51938	-1.02493600
H	2.805039	0.80864	-1.14531600
H	-2.436441	0.983108	-0.18989300
S	0.694498	1.942079	-0.17417400
O	-0.138896	2.925328	-0.84813500
O	-0.019689	1.193082	0.84515600
O	1.36457	1.030611	-1.13478100
N	-2.679492	1.989406	-0.05151000
H	-1.843595	2.505627	-0.37355900
C	-2.919005	2.254361	1.38334800
H	-3.741684	1.624709	1.70746700
H	-3.158386	3.307463	1.50981100
H	-2.013683	2.001419	1.92487400
C	-3.849207	2.275795	-0.90336600
H	-4.664158	1.637016	-0.57420600
H	-3.593	2.049925	-1.93407500
H	-4.11901	3.324154	-0.80601400
H	0.957348	-0.879998	-0.31470200
S	-3.228845	-1.403595	0.07805900
O	-2.280319	-0.626985	-0.76294300
O	-2.518867	-2.325838	0.94042700
O	-4.174091	-0.520806	0.73340500
N	0.257864	-1.521868	0.06824800
H	-0.641641	-1.01845	0.00784100
C	0.581962	-1.827318	1.47965200
H	1.529236	-2.357702	1.50119700
H	-0.229104	-2.428467	1.87899000
H	0.669424	-0.888002	2.01430200
C	0.162044	-2.725625	-0.78214100
H	1.12611	-3.223809	-0.78463500
H	-0.10693	-2.414953	-1.78720400
H	-0.616147	-3.359491	-0.36700100
C	1.999144	2.822555	0.62531000
H	1.545409	3.507227	1.33538700
H	2.631878	2.09717	1.13094200
H	2.55264	3.368761	-0.13335400
C	-4.158975	-2.388006	-1.06398300
H	-4.859424	-2.984941	-0.48756400
H	-4.687193	-1.723513	-1.74090200
H	-3.470554	-3.026204	-1.610088

Table S18: Geometry of DMA<sub>2</sub>SA<sub>2</sub>MSA. Units are Å.

Atom	X	Y	Z
S	3.969449	-0.435674	0.07006900
C	3.754733	-1.424963	1.51286800
H	4.013181	-0.80228	2.36454900
H	2.713245	-1.733989	1.55739100
H	4.424155	-2.276045	1.43836900
O	5.339819	-0.083926	-0.07880100
O	2.996309	0.627099	0.12821500
O	3.603216	-1.402198	-1.08294700
H	2.646192	-1.701976	-0.99022700
N	0.853806	2.290418	0.00221000
H	1.081774	1.290806	0.04234200
C	1.399866	2.964692	1.19668100
H	1.141423	4.018977	1.14993100
H	2.476217	2.827245	1.20734000
H	0.954893	2.515456	2.07965900
C	1.387507	2.812944	-1.27469500
H	1.095108	3.854714	-1.37242300
H	0.965126	2.22306	-2.08217800
H	2.467584	2.707161	-1.26363600
S	0.085829	-1.351423	-0.34372500
O	-1.18565	-2.048058	-0.33551000
O	1.22798	-2.217573	-0.53467400
O	0.080428	-0.196465	-1.24388200
H	-1.457758	0.384639	-1.39295800
O	0.293855	-0.756527	1.10282900
H	-0.499761	-0.182314	1.27572100
S	-2.543052	1.484497	0.08877700
O	-2.397569	0.687919	-1.27248200
O	-1.887339	0.650533	1.10634500
O	-1.859088	2.75055	-0.08122000
H	-0.18245	2.399549	-0.00512700
O	-3.968668	1.540338	0.27778800
H	-4.095913	-0.396666	0.26681700
N	-3.775735	-1.374629	0.19147900
H	-2.755613	-1.342149	-0.00760700
C	-4.427888	-2.036371	-0.95624000
H	-5.495964	-2.110787	-0.77222100
H	-3.992708	-3.024684	-1.07469200
H	-4.235408	-1.438154	-1.84153000
C	-3.948537	-2.067397	1.48372100
H	-5.007187	-2.141559	1.71615400
H	-3.431742	-1.490231	2.24435800
H	-3.506948	-3.056679	1.40292

Table S19: Geometry of DMA<sub>2</sub>SA MSA<sub>2</sub>. Units are Å.

Atom	X	Y	Z
S	4.026215	-0.02083	0.14005500
C	4.761201	-1.601311	0.39052400
H	3.961624	-2.337698	0.40619400
H	5.455998	-1.785343	-0.42256300
H	5.277626	-1.568062	1.34534900
O	5.038949	0.96772	-0.03205900
O	3.056465	0.178126	1.18765600
O	3.290735	-0.178342	-1.20988800
H	2.498795	-0.835064	-1.12345900
N	-2.936263	-1.879587	0.70823800
H	-2.236356	-2.071448	-0.04424000
C	-4.298494	-2.109808	0.19545700
H	-5.017498	-1.861705	0.97174900
H	-4.401488	-3.152925	-0.09171400
H	-4.442419	-1.465707	-0.66683800
C	-2.57711	-2.687342	1.88831500
H	-3.254116	-2.449859	2.70478600
H	-1.55378	-2.444345	2.15765200
H	-2.655717	-3.740946	1.63366300
S	-2.855963	1.425074	-0.19443500
O	-1.710474	2.318549	-0.07116600
O	-2.654762	0.39717	-1.22426900
H	-1.061543	0.105373	-1.62452400
O	-3.281632	0.838305	1.07127500
S	0.054977	-1.397244	-0.65944000
O	-0.110715	-0.188167	-1.65780000
O	-0.187654	-0.86503	0.66997900
O	-0.913701	-2.413879	-1.02753700
H	-2.851014	-0.869768	0.93128100
O	1.432831	-1.816989	-0.88474100
H	1.208381	0.801167	0.59962200
N	0.866804	1.765438	0.54257100
H	-0.124509	1.735888	0.23691400
C	1.655018	2.528317	-0.44594700
H	2.692655	2.562842	-0.12309400
H	1.240127	3.530596	-0.51222500
H	1.581194	2.024922	-1.40496300
C	0.905459	2.334	1.90394300
H	1.934667	2.332444	2.25005700
H	0.289349	1.712827	2.54705400
H	0.503948	3.342769	1.86873400
C	-4.195047	2.429365	-0.75774200
H	-4.376201	3.194853	-0.00944400
H	-3.906655	2.873439	-1.70540600
H	-5.067018	1.793749	-0.878027

Table S20: Geometry of DMA<sub>3</sub>SA<sub>2</sub>MSA. Units are Å.

Atom	X	Y	Z
S	4.256833	0.012986	0.01001500
C	5.785718	0.314961	0.84473200
H	6.067355	-0.594149	1.36687400
H	6.52742	0.573385	0.09503700
H	5.641231	1.132312	1.54429700
O	3.270261	-0.300076	1.05470300
O	4.476925	-1.097392	-0.89211700
O	3.917677	1.270761	-0.66586100
N	1.788212	-2.319323	-0.10400200
H	2.37113	-1.698108	0.49230200
C	1.372418	-1.529642	-1.28812900
H	0.630606	-2.100825	-1.83953200
H	2.254416	-1.320291	-1.88511000
H	0.924928	-0.604979	-0.93330800
C	2.525881	-3.54827	-0.46529500
H	1.877894	-4.166372	-1.08081300
H	2.788416	-4.081569	0.44317200
H	3.422745	-3.256838	-1.00297500
S	-1.913319	1.938573	-0.31785000
O	-3.176694	1.922064	-1.03144400
O	-1.247963	3.207422	-0.23971900
O	-2.040114	1.245138	0.97229400
H	-1.18203	-0.099828	1.19583900
O	-0.898093	1.051026	-1.16379200
H	-1.248854	0.112212	-1.19958700

Table S21: Geometry of DMA<sub>3</sub>SA<sub>2</sub>MSA (contunued). Units are Å.

Atom	X	Y	Z
S	-1.658211	-1.980478	0.33549200
O	-0.72373	-0.987842	1.13804200
O	-1.923575	-1.316257	-0.94932800
O	-0.85207	-3.169212	0.21999300
H	0.929228	-2.580378	0.39795300
O	-2.885232	-2.129693	1.09451200
H	-3.878682	-0.823559	0.55783200
N	-4.539066	-0.196006	0.05392600
H	-3.96609	0.502938	-0.46390700
C	-5.36656	0.549663	1.02067300
H	-5.932171	-0.152427	1.62709500
H	-6.041248	1.204357	0.47550100
H	-4.70139	1.140899	1.64290600
C	-5.296857	-1.026774	-0.90039500
H	-5.898671	-1.742296	-0.34667000
H	-4.580994	-1.550867	-1.52662400
H	-5.934613	-0.387493	-1.50497300
N	1.53713	2.332055	-0.03080700
C	1.806264	3.77865	-0.17433900
C	1.177938	1.945094	1.35404600
H	2.403696	1.811297	-0.32103000
H	0.299307	2.509249	1.65190700
H	2.028562	2.157003	1.99549400
H	0.978437	0.878514	1.37412500
H	0.911731	4.32527	0.10598800
H	2.065936	3.9857	-1.20789900
H	2.643016	4.033488	0.46997500
H	0.761953	2.069382	-0.646246
H	2.028562	2.157003	1.99549400
H	0.978437	0.878514	1.37412500
H	0.911731	4.32527	0.10598800
H	2.065936	3.9857	-1.20789900
H	2.643016	4.033488	0.46997500
H	0.761953	2.069382	-0.646246