

Supplementary material for:

On the formation of sulphuric acid – amine clusters in varying atmospheric conditions and its influence on atmospheric new particle formation

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This supplementary material contains the following:

Table S1. Electronic energies of formation at the B3LYP/CBSB7//RI-CC2/aug-cc-pV(T+d)Z level.

Table S2. Cartesian coordinates for the most stable structure of each cluster, optimized at the B3LYP/CBSB7 level.

Figure S1. Most stable conformers of the clusters a) A₂D₂, b) A₂T₂ and c) A₂D₁T₁.

Table S1. Electronic energies of formation at the B3LYP/CBSB7//RI-CC2/aug-cc-pV(T+d)Z level.

Cluster	ΔE_{elec}
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_3\text{N}$	-28.49
$(\text{H}_2\text{SO}_4)_2 \cdot (\text{CH}_3)_3\text{N}$	-57.86
$(\text{H}_2\text{SO}_4)_3 \cdot (\text{CH}_3)_3\text{N}$	-81.61
$\text{H}_2\text{SO}_4 \cdot ((\text{CH}_3)_3\text{N})_2$	-45.79
$(\text{H}_2\text{SO}_4)_2 \cdot ((\text{CH}_3)_3\text{N})_2$	-92.65
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{CH}_3)_3\text{N}$	-44.96
$(\text{H}_2\text{SO}_4)_2 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{CH}_3)_3\text{N}$	-91.57
$\text{H}_2\text{SO}_4 \cdot \text{H}_2\text{O}$	-13.07
$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_2$	-25.78
$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_3$	-39.54
$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_4$	-52.62
$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_5$	-63.03
$(\text{H}_2\text{SO}_4)_2 \cdot \text{H}_2\text{O}$	-34.07
$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_2$	-50.13
$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_3$	-63.47
$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_4$	-76.04
$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_5$	-92.61
$(\text{CH}_3)_2\text{NH} \cdot \text{H}_2\text{O}$	-7.91
$(\text{CH}_3)_2\text{NH} \cdot (\text{H}_2\text{O})_2$	-17.60
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot \text{H}_2\text{O}$	-42.48
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{H}_2\text{O})_2$	-55.50
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{H}_2\text{O})_3$	-67.49
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{H}_2\text{O})_4$	-79.93
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{H}_2\text{O})_5$	-91.91
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_3\text{N} \cdot \text{H}_2\text{O}$	-40.49
$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_3\text{N} \cdot (\text{H}_2\text{O})_2$	-51.96

Table S2. Cartesian coordinates for the most stable structure of each cluster, optimized at the B3LYP/CBSB7 level.

(CH₃)₃N

N	-0.000078	-0.000227	-0.370144
C	-1.286535	-0.525973	0.060570
C	0.187520	1.376715	0.060469
C	1.099073	-0.850592	0.060547
H	-0.619763	2.000529	-0.331500
H	1.132765	1.761526	-0.330587
H	0.202339	1.488780	1.162500
H	-2.092524	0.099607	-0.331299
H	-1.391503	-0.568295	1.162582
H	-1.423349	-1.537276	-0.330670
H	1.190083	-0.917987	1.162532
H	2.042696	-0.464116	-0.332907
H	0.959452	-1.862077	-0.329160

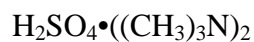
H₂O

O	0.000000	0.000000	0.118741
H	0.000000	0.757218	-0.474964
H	0.000000	-0.757218	-0.474964

H₂SO₄•(CH₃)₃N

S	1.514143	-0.142179	0.033356
O	2.635258	-0.973264	0.395003
O	0.468014	-0.068746	1.106066
O	0.890714	-0.333270	-1.268352
H	-0.865966	-0.014992	0.512592
O	2.096918	1.395786	-0.057381
H	2.844734	1.438163	0.552891
N	-1.875319	0.012207	0.064388
C	-1.882598	1.156266	-0.889229

C	-2.841183	0.197411	1.175413
C	-2.058930	-1.289382	-0.635375
H	-2.612675	1.129787	1.690455
H	-2.737374	-0.630798	1.875510
H	-3.860594	0.228640	0.785581
H	-1.674514	2.071300	-0.335819
H	-2.857646	1.225997	-1.375930
H	-1.089001	0.989732	-1.614677
H	-3.035061	-1.312788	-1.124405
H	-1.990029	-2.091047	0.099084
H	-1.251902	-1.394396	-1.357242



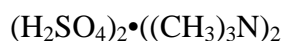
S	0.060684	-0.860522	-0.026741
O	-0.834161	-1.585562	-0.907018
O	-0.828875	-0.170216	1.109327
O	0.724335	0.294034	-0.748131
H	-1.720075	0.113593	0.707833
O	1.064494	-1.626657	0.702508
H	2.057665	0.425123	-0.349522
N	3.142260	0.529597	-0.037721
C	3.144260	0.640935	1.445145
C	3.671178	1.748120	-0.693191
C	3.833612	-0.703865	-0.496874
H	3.081504	2.606536	-0.372638
H	3.578966	1.637624	-1.773286
H	4.719660	1.899441	-0.425306
H	2.564754	1.519014	1.729050
H	4.169384	0.734979	1.811744
H	2.660372	-0.247444	1.845797
H	4.886587	-0.673288	-0.205899
H	3.749301	-0.766848	-1.581450

H	3.324549	-1.555428	-0.050329
N	-3.222483	0.496832	0.058472
C	-2.984006	0.987465	-1.304581
C	-3.910451	1.495607	0.877388
C	-3.944439	-0.781451	0.042018
H	-3.319840	2.413896	0.910109
H	-4.021641	1.121755	1.897562
H	-4.910897	1.738403	0.483594
H	-2.383624	1.898750	-1.263587
H	-3.926993	1.207412	-1.830600
H	-2.424450	0.234371	-1.858868
H	-4.940968	-0.683992	-0.417894
H	-4.065873	-1.142483	1.065559
H	-3.355032	-1.511718	-0.512205

$(\text{H}_2\text{SO}_4)_2 \cdot (\text{CH}_3)_3\text{N}$

S	-2.347013	-0.789582	-0.021550
O	-2.145744	-0.099343	1.390838
O	-1.077157	-1.368807	-0.418152
O	-2.668928	0.417455	-0.987946
O	-3.516397	-1.594383	0.059716
H	-1.284479	0.399651	1.399904
H	-1.873290	1.008606	-1.069465
S	0.604610	1.776928	-0.042219
O	1.100910	3.251540	0.410867
O	0.226215	1.145267	1.221997
O	1.774944	1.126764	-0.658050
O	-0.492895	2.003109	-0.982369
H	1.026250	3.832278	-0.359407
H	1.986708	-0.424370	-0.236577
N	2.306663	-1.413404	-0.036521
C	1.895685	-2.244339	-1.208877
C	1.646685	-1.867023	1.226654

C	3.787226	-1.331155	0.104123
H	0.572910	-1.883330	1.058118
H	1.882631	-1.154995	2.015083
H	2.016691	-2.861076	1.481839
H	0.811396	-2.207221	-1.288096
H	2.237263	-3.269232	-1.057963
H	2.350151	-1.825572	-2.105720
H	4.191429	-2.327008	0.288898
H	4.023817	-0.669716	0.935870
H	4.205166	-0.919431	-0.813137



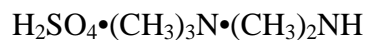
S	1.116615	1.624825	-0.558032
O	1.510216	0.498661	0.374462
O	1.101108	1.161781	-1.937844
O	1.822286	2.845053	-0.254846
H	-1.186133	-0.857724	-1.907509
O	-0.416197	1.940563	-0.136038
H	-0.919483	1.085391	-0.179179
N	-1.102623	-1.156864	-2.925514
C	0.272085	-1.708768	-3.126994
C	-1.335058	0.060733	-3.755292
C	-2.157061	-2.194688	-3.112201
H	-0.575311	0.795046	-3.492270
H	-2.325487	0.452833	-3.526794
H	-1.274172	-0.204728	-4.811880
H	0.985034	-0.914083	-2.915674
H	0.365123	-2.058085	-4.156732
H	0.419108	-2.526221	-2.424420
H	-2.102852	-2.590349	-4.127270
H	-3.129750	-1.737825	-2.936554
H	-2.001262	-2.980031	-2.374233
S	-1.116615	-1.624825	0.558032

O	-1.822286	-2.845053	0.254846
O	-1.101108	-1.161781	1.937844
O	-1.510216	-0.498661	-0.374462
H	1.186133	0.857724	1.907509
O	0.416197	-1.940563	0.136038
H	0.919483	-1.085391	0.179179
N	1.102623	1.156864	2.925514
C	2.157061	2.194688	3.112201
C	1.335058	-0.060733	3.755292
C	-0.272085	1.708768	3.126994
H	2.325487	-0.452833	3.526794
H	0.575311	-0.795046	3.492270
H	1.274172	0.204728	4.811880
H	3.129750	1.737825	2.936554
H	2.102852	2.590349	4.127270
H	2.001262	2.980031	2.374233
H	-0.365123	2.058085	4.156732
H	-0.985034	0.914083	2.915674
H	-0.419108	2.526221	2.424420

$(\text{H}_2\text{SO}_4)_3 \cdot (\text{CH}_3)_3\text{N}$

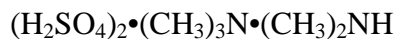
S	0.409195	-0.308978	1.130211
O	0.691222	0.898985	0.294027
O	1.536815	-0.648835	1.976671
O	0.241289	-1.519267	0.058886
O	-0.889923	-0.227674	1.772233
H	-0.598902	1.955976	-0.002102
H	1.112280	-1.629919	-0.402057
S	3.796732	-0.472486	-0.585522
O	4.086479	-0.669916	0.956986
O	5.041706	-0.493157	-1.262630
O	3.225516	1.006401	-0.670879
O	2.727511	-1.379481	-0.967924

H	3.228848	-0.738202	1.444567
H	2.288240	1.014839	-0.344985
N	-1.202783	2.798313	-0.161751
C	-1.576327	2.808113	-1.610951
C	-0.359783	3.973169	0.207800
C	-2.403965	2.673137	0.722767
H	0.529120	3.982476	-0.420819
H	-0.064588	3.879101	1.251300
H	-0.933380	4.888193	0.059906
H	-0.663297	2.835305	-2.204190
H	-2.180810	3.692457	-1.814441
H	-2.135022	1.900004	-1.824338
H	-3.020259	3.565325	0.608555
H	-2.067143	2.571482	1.752777
H	-2.949881	1.782432	0.423758
S	-3.277789	-1.326968	-0.477924
O	-2.743754	-0.059729	-0.934522
O	-2.225531	-2.460325	-0.828837
O	-4.551746	-1.785681	-0.904629
H	-1.319276	-2.152252	-0.601738
O	-3.287802	-1.309448	1.108437
H	-2.430454	-0.941989	1.437575



S	-0.32985	-0.71013	-0.18161
O	-1.42556	-1.03498	-1.11991
O	0.53721	0.36934	-0.98340
O	0.54437	-1.80873	0.17322
H	1.46492	0.42418	-0.56365
O	-0.87373	0.01422	1.00853
N	3.01102	0.42629	0.07797
C	2.87586	0.23372	1.52783
C	3.70740	1.67485	-0.23586

C	3.66194	-0.73005	-0.55078
H	3.16803	2.51651	0.20418
H	3.74112	1.81540	-1.31850
H	4.73989	1.68244	0.14946
H	2.32257	1.07187	1.95627
H	3.85757	0.16517	2.02320
H	2.30955	-0.67877	1.71271
H	4.68520	-0.88074	-0.17157
H	3.70844	-0.57717	-1.63117
H	3.06454	-1.62046	-0.35501
N	-3.27058	0.40266	0.08570
H	-2.40118	0.41655	0.71019
H	-2.84546	-0.23007	-0.64219
C	-4.41745	-0.23795	0.76201
C	-3.52207	1.74520	-0.48133
H	-5.24034	-0.36874	0.05801
H	-4.09716	-1.20997	1.13446
H	-4.74552	0.38216	1.59703
H	-4.31568	1.69155	-1.22765
H	-3.81205	2.43227	0.31440
H	-2.60218	2.09372	-0.94887



S	-0.54945	-1.85844	-0.17851
O	-0.88638	-0.83536	0.87871
O	0.81566	-2.35384	0.01574
O	-0.56837	-1.02271	-1.55295
O	-1.58692	-2.84337	-0.33841
H	-2.27752	-0.10824	0.52112
H	0.07341	-0.25815	-1.48253
S	1.16608	2.01325	-0.16978
O	2.26084	1.71356	0.77742
O	1.07514	3.36938	-0.62536

O	-0.21527	1.78007	0.68604
O	1.12460	0.96817	-1.22462
H	2.77204	0.17618	0.57161
H	-0.25942	0.82268	0.91004
N	-3.20081	0.37130	0.29266
C	-3.03145	1.05518	-1.02660
C	-3.46037	1.34925	1.38835
C	-4.22078	-0.71640	0.23507
H	-2.63389	2.05783	1.41493
H	-3.51425	0.81027	2.33338
H	-4.40219	1.86574	1.19860
H	-2.23496	1.78986	-0.92715
H	-3.97129	1.53615	-1.30114
H	-2.74297	0.31050	-1.76502
H	-5.18653	-0.29427	-0.04554
H	-4.28428	-1.18691	1.21496
H	-3.89128	-1.45927	-0.48906
C	3.76124	-1.38494	1.55511
H	4.66215	-0.80547	1.75667
H	3.09181	-1.32955	2.41225
H	4.02176	-2.42601	1.36447
N	3.06424	-0.82234	0.37426
C	3.85483	-0.83355	-0.88334
H	4.09396	-1.86173	-1.15506
H	3.24876	-0.36576	-1.65628
H	4.77025	-0.26037	-0.73646
H	2.17939	-1.35753	0.22019

H₂SO₄•H₂O

S	-0.586942	-0.098902	0.112848
O	-0.867917	1.435334	-0.312959
O	0.329528	-0.615636	-1.060503
O	0.194987	0.004056	1.312958

O	-1.818404	-0.815421	0.046021
H	-1.596971	1.440636	-0.950575
H	1.286153	-0.407978	-0.836300
H	2.316922	-0.001491	0.825836
O	2.700325	-0.043009	-0.063098
H	3.076818	0.828665	-0.223879

$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_2$

S	-0.993997	-0.169099	-0.090923
O	-0.358806	1.075492	-0.777581
O	-1.275468	0.352789	1.416705
O	-2.247438	-0.427772	-0.722252
O	-0.011897	-1.206513	0.084110
H	0.614465	1.240178	-0.475565
H	-2.113611	0.837898	1.409131
H	1.875818	-1.393289	0.204840
O	2.799901	-1.104995	0.113954
H	3.132528	-1.555466	-0.668711
H	2.196697	1.873765	0.770083
O	2.056997	1.453135	-0.084050
H	2.491733	0.565399	-0.032099

$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_3$

O	-1.621864	-1.440882	-1.057064
H	-1.895063	-0.613352	-1.479258
H	-2.048691	-1.392126	-0.185293
S	1.271053	0.019913	0.152541
O	2.676279	0.117623	0.327752
O	0.984532	-1.220251	-0.769446
O	0.814417	1.262549	-0.724206
O	0.393358	-0.047472	1.310444
H	-0.007572	-1.370694	-0.875063
H	-0.172971	1.363002	-0.704511

O	-1.893915	1.395658	-0.750167
H	-2.244546	1.073342	0.106295
H	-2.326099	2.231096	-0.951377
O	-2.294337	-0.208821	1.391029
H	-2.773396	-0.279326	2.221575
H	-1.336270	-0.197781	1.600247

$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_4$

O	-2.585774	0.042980	0.042402
H	-2.236617	-0.762505	-0.493915
H	-2.186162	0.884037	-0.399337
H	-2.169956	-0.023472	0.983367
O	-1.490548	-1.907551	-1.176628
H	-0.590724	-1.877044	-0.771726
H	-1.352552	-1.827942	-2.125862
O	-1.384595	1.989076	-1.067640
H	-0.501672	1.584005	-1.253647
H	-1.203843	2.755442	-0.513377
O	-1.353498	-0.052117	2.268930
H	-1.171080	-0.936784	2.603887
H	-0.472233	0.313106	2.013194
S	1.238764	-0.018602	-0.011668
O	2.851324	-0.184691	-0.003553
O	0.776581	-1.392597	0.168921
O	0.887188	0.568408	-1.312840
O	0.902896	0.872616	1.108428
H	3.236018	0.699800	-0.080054

$\text{H}_2\text{SO}_4 \cdot (\text{H}_2\text{O})_5$

S	1.363916	-0.327819	-0.250819
O	2.159141	0.886199	-0.349595
O	0.497943	-0.563773	-1.424881
O	0.654361	-0.488117	1.021868

O	2.402010	-1.578278	-0.238785
H	3.015074	-1.454036	-0.977118
O	-1.804928	0.537895	-1.397677
H	-2.410075	-0.114916	-0.874694
H	-0.882070	0.111143	-1.476559
H	-1.705589	1.418697	-0.875501
O	-3.166081	-1.140294	-0.086506
H	-3.823563	-0.819734	0.538196
H	-2.518869	-1.685201	0.440513
O	-1.535413	2.659875	-0.040255
H	-0.742316	2.625580	0.565080
H	-1.488055	3.498847	-0.508115
O	0.636208	2.423537	1.472699
H	1.354781	2.206002	0.852142
H	0.528550	1.581030	1.936283
O	-1.300585	-2.381117	1.307480
H	-0.946679	-3.214362	0.982183
H	-0.545096	-1.755363	1.295915

$(\text{H}_2\text{SO}_4)_2 \cdot \text{H}_2\text{O}$

S	1.807805	-0.395575	-0.017867
O	2.445773	0.998549	-0.206492
O	1.101151	-0.448315	1.246473
O	3.108645	-1.302278	0.067956
O	1.112161	-0.838233	-1.196431
H	1.735349	1.766956	-0.089492
H	3.557441	-1.142162	0.912701
S	-2.156048	-0.088300	-0.012054
O	-1.660314	-0.698395	1.364851
O	-3.572822	-0.117054	0.000833
O	-1.668669	-1.144547	-1.089128
O	-1.431598	1.145541	-0.247365
H	-0.682557	-0.611028	1.437610

H	-0.702175	-1.048935	-1.246163
O	0.711201	2.784046	0.063371
H	-0.155398	2.329589	0.095577
H	0.655023	3.413094	-0.664067

$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_2$

S	-2.233851	-0.072187	0.017212
O	-1.985597	-1.570023	-0.401038
O	-1.482672	0.775580	-0.899544
O	-1.572840	0.043904	1.448064
O	-3.630376	0.114464	0.165980
H	-1.014532	-1.742763	-0.509262
H	-0.583268	-0.000040	1.384339
S	1.621266	-0.802527	-0.038865
O	0.713437	-1.867876	-0.440343
O	2.911768	-1.502451	0.617420
O	1.111734	0.028528	1.070023
O	2.118863	0.014094	-1.158733
H	3.213500	-2.205617	0.023176
O	0.692036	2.122213	-1.360056
H	-0.228247	1.749037	-1.237787
H	0.976935	2.536521	-0.460456
H	1.292402	1.298894	-1.443336
O	1.424189	2.758023	0.972655
H	1.479088	1.838842	1.301701
H	2.261153	3.188897	1.172656

$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_3$

S	2.425385	0.033044	0.143006
O	2.404108	-1.392950	-0.529560
O	3.776783	0.358691	0.428714
O	1.681271	-0.183522	1.521899
O	1.605747	0.912097	-0.675246

H	1.472267	-1.636835	-0.764655
H	0.709541	-0.314041	1.367578
S	-1.317271	-1.226429	-0.270348
O	-0.221740	-1.958002	-0.885995
O	-2.350487	-2.331877	0.302798
O	-2.084469	-0.395761	-1.207081
O	-0.946457	-0.497919	0.959218
H	-2.536646	-2.965430	-0.405624
O	-2.251981	2.113274	-0.651790
H	-2.448169	2.034113	0.345986
H	-1.316141	2.549196	-0.781060
H	-2.208738	1.155448	-0.976793
O	0.046689	3.088226	-0.880142
H	0.711287	2.382552	-0.719040
H	0.303917	3.522347	-1.699587
O	-2.537112	1.571565	1.824472
H	-2.011459	0.747212	1.790054
H	-3.384506	1.349013	2.222321

$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_4$

S	2.493506	-0.801735	0.106421
O	1.880190	-0.402524	1.507595
O	2.090094	0.203022	-0.864646
O	1.751985	-2.143310	-0.263997
O	3.866120	-1.104179	0.304638
H	0.936022	-0.113114	1.394432
H	0.784622	-1.966697	-0.405370
S	-1.474901	-0.324705	0.041280
O	-0.655763	0.370886	1.056453
O	-2.804815	-0.695731	0.818264
O	-0.882662	-1.587732	-0.419371
O	-1.848855	0.567446	-1.067474
H	-3.233967	-1.467508	0.349009

O	-0.945502	2.959341	-0.902248
H	-1.117453	3.124561	0.087674
H	-1.318997	2.028721	-1.071733
H	0.079562	2.932497	-1.065762
O	-3.474137	-2.830651	-0.603764
H	-3.884983	-2.674605	-1.460889
H	-2.531169	-2.955139	-0.790466
O	1.542635	2.812774	-1.206417
H	1.848425	1.899893	-1.006831
H	1.943077	3.056272	-2.046713
O	-1.328669	2.977138	1.629092
H	-2.198405	3.120987	2.015411
H	-1.129379	2.025326	1.733032

$(\text{H}_2\text{SO}_4)_2 \cdot (\text{H}_2\text{O})_5$

S	2.608425	-0.056711	-0.170909
O	1.906865	-0.503940	1.034290
O	4.147258	-0.402476	0.167794
O	2.557295	1.390536	-0.398221
O	2.269213	-0.828427	-1.374666
H	4.694534	-0.105319	-0.573822
S	-2.517837	-0.204884	-0.005299
O	-1.737524	-0.425405	-1.232868
O	-3.797847	-1.167271	-0.236292
O	-3.015137	1.156386	0.132518
O	-1.843956	-0.697622	1.209306
H	-4.432328	-0.996712	0.475097
O	0.109374	-2.239636	-1.374443
H	0.969279	-1.719209	-1.480662
H	0.111973	-2.563132	-0.370339
H	-0.647847	-1.574824	-1.425701
O	0.527547	2.835929	0.366541
H	1.355018	2.387572	0.021660

H	0.225425	2.241727	1.172984
H	-0.194060	2.810717	-0.368557
O	-0.001304	1.215124	2.208714
H	-0.790205	0.666483	2.038494
H	0.748241	0.604945	2.082135
O	-1.306842	2.670977	-1.390512
H	-2.087173	2.320188	-0.912635
H	-1.130346	1.992005	-2.053690
O	0.122121	-2.699458	1.080722
H	-0.654830	-2.169372	1.344666
H	0.886397	-2.147296	1.326636

$(\text{CH}_3)_2\text{NH}\cdot\text{H}_2\text{O}$

N	-0.487268	0.470159	0.000000
C	0.114726	0.995917	1.223799
C	0.114726	0.995917	-1.223799
H	-0.413768	0.593684	2.090098
H	0.108436	2.095695	1.283482
H	1.154267	0.661555	1.286433
H	0.108436	2.095695	-1.283482
H	-1.483898	0.659207	0.000000
H	-0.413768	0.593684	-2.090098
H	1.154267	0.661555	-1.286433
O	0.114726	-2.359011	0.000000
H	-0.172092	-1.424515	0.000000
H	1.074485	-2.306584	0.000000

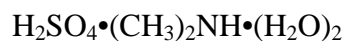
$(\text{CH}_3)_2\text{NH}\cdot(\text{H}_2\text{O})_2$

N	-0.776204	-0.022529	-0.000001
C	-1.575452	-0.075234	1.221964
C	-1.575487	-0.075129	-1.221947
H	-0.908620	-0.097526	2.086135
H	-2.239380	-0.953091	1.271252

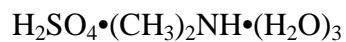
H	-2.200045	0.820376	1.297229
H	-2.239415	-0.952984	-1.271291
H	-0.104360	-0.789673	-0.000041
H	-0.908681	-0.097344	-2.086140
H	-2.200085	0.820485	-1.297115
O	1.604780	1.417235	0.000043
H	1.655648	2.374760	0.000065
H	0.650814	1.163936	0.000034
O	1.892210	-1.300670	-0.000105
H	2.145785	-0.361343	-0.000012
H	2.711477	-1.800230	0.000281

$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot \text{H}_2\text{O}$

S	1.466548	-0.077051	-0.130798
O	0.498244	-0.947766	-0.829561
O	0.795591	0.734309	0.905358
O	2.357299	-1.175142	0.693007
O	2.378841	0.655020	-0.976865
H	-0.994282	-0.629152	-0.408525
H	3.196664	-0.745365	0.905017
N	-1.955776	-0.293666	-0.086546
H	-1.867093	0.748163	-0.103238
O	-1.222863	2.352718	0.148702
H	-0.989085	2.947340	-0.570610
H	-0.368130	1.989065	0.475395
C	-2.998983	-0.749426	-1.033432
H	-3.971428	-0.358027	-0.732723
H	-3.028506	-1.838928	-1.042419
H	-2.749848	-0.389404	-2.031017
C	-2.150433	-0.730957	1.320063
H	-3.088849	-0.330818	1.704933
H	-1.309368	-0.355014	1.899528
H	-2.164803	-1.820189	1.357323



S	1.595632	-0.435792	-0.185678
O	1.512572	0.304226	1.329564
O	2.983160	-0.781352	-0.346900
O	1.049181	0.607012	-1.054092
O	0.670834	-1.579659	-0.067390
H	2.266442	-0.029177	1.833036
N	-1.868553	-0.684361	-0.058557
H	-1.725754	0.085230	0.651771
H	-0.894922	-1.076373	-0.185018
O	-1.169703	1.317106	1.667509
H	-0.266102	1.025006	1.873493
H	-1.026992	2.040184	1.020193
O	-0.546543	2.738110	-0.570035
H	0.168009	2.101749	-0.783627
H	-0.192072	3.614436	-0.742668
C	-2.740962	-1.741595	0.504405
H	-2.279274	-2.128026	1.412038
H	-2.847764	-2.550280	-0.218784
H	-3.720260	-1.324092	0.739190
C	-2.349157	-0.091606	-1.333818
H	-1.688217	0.730610	-1.599248
H	-3.364733	0.282147	-1.198488
H	-2.333888	-0.852549	-2.113918



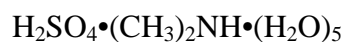
S	1.185230	-0.529734	-0.208150
O	1.251588	1.090367	0.019374
O	0.961176	-1.117763	1.110762
O	-0.010508	-0.638520	-1.083729
O	2.433710	-0.908304	-0.849722
H	2.199843	1.324503	0.186912

N	-1.931530	1.100917	-0.113439
C	-1.654470	2.522885	0.207493
C	-3.211448	0.850150	-0.827011
H	-1.149647	0.688922	-0.664598
H	-1.908948	0.507291	0.769008
H	-3.297149	-0.223025	-0.994222
H	-4.040220	1.200362	-0.211509
H	-3.207220	1.382768	-1.778136
H	-0.674592	2.577820	0.676053
H	-1.651715	3.109246	-0.711494
H	-2.425310	2.895668	0.882187
H	3.821103	0.373327	-0.342902
O	3.950583	1.177521	0.192296
H	4.288294	0.851586	1.033248
H	-0.740014	-0.834679	1.895444
O	-1.710734	-0.713798	1.887708
H	-2.004831	-1.454404	1.322603
H	-2.102969	-3.187616	-0.551582
O	-2.133793	-2.239920	-0.393336
H	-1.290262	-1.877328	-0.736255

$\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH} \cdot (\text{H}_2\text{O})_4$

S	1.324850	-0.322387	-0.250447
O	2.482838	-0.507036	-1.336443
O	1.385900	-1.464714	0.664353
O	1.558586	0.971272	0.415142
O	0.086979	-0.306004	-1.059781
H	3.319496	-0.158612	-0.935087
N	-1.646753	1.422701	0.158814
C	-1.418932	2.799500	-0.344989
C	-1.477729	1.264964	1.630004
H	-2.592063	1.068105	-0.123163
H	-0.966216	0.784167	-0.322247

H	-0.464553	1.561371	1.895222
H	-2.212337	1.885334	2.144595
H	-1.620719	0.212844	1.878346
H	-1.598222	2.810965	-1.419227
H	-2.101386	3.490696	0.150137
H	-0.384804	3.075276	-0.143350
H	-1.965176	-2.177960	-0.042123
O	-2.249388	-1.976478	-0.956487
H	-1.431043	-1.641525	-1.355854
H	-4.685621	-0.104082	-0.321662
O	-3.864895	0.134845	-0.760846
H	-3.370892	-0.716256	-0.911757
H	-0.188857	-1.946254	1.320272
O	-1.125169	-2.098831	1.581136
H	-1.111100	-2.853125	2.176990
H	3.515383	1.168642	0.500428
O	4.340884	0.764798	0.176646
H	4.641877	0.210094	0.904086



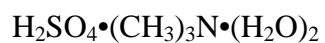
S	0.522811	-0.330891	-0.716722
O	1.748533	-0.003948	-1.623027
O	0.098136	0.947282	-0.057062
O	-0.523213	-0.806175	-1.628031
O	0.920770	-1.326681	0.292721
H	2.582038	0.298449	-1.064299
N	-2.609305	0.763650	0.212267
C	-3.051188	1.552305	-0.966074
C	-3.183508	1.177238	1.519372
H	-2.815254	-0.237113	0.038048
H	-1.558846	0.820949	0.252299
H	-2.783752	0.496262	2.268305
H	-2.886289	2.204162	1.731366

H	-4.271014	1.109080	1.477129
H	-4.131545	1.465238	-1.082854
H	-2.540111	1.155490	-1.841459
H	-2.775847	2.596493	-0.822775
H	3.850539	-0.005936	0.404436
O	3.714177	0.732914	-0.228967
H	3.352619	1.486436	0.284127
H	1.329483	2.137184	0.628218
O	2.103533	2.701317	0.822065
H	2.074620	3.386834	0.147021
H	3.913809	-2.295510	0.817963
O	3.537461	-1.537841	1.276569
H	2.585860	-1.568138	1.061699
H	-1.868393	-1.750950	-1.079546
O	-2.706877	-1.955571	-0.602344
H	-3.233549	-2.514726	-1.179865
H	-1.933038	-2.053574	1.308795
O	-1.517055	-1.464066	1.952484
H	-0.586723	-1.457012	1.678038



S	1.59878	-0.33855	-0.11442
O	2.83076	-0.70857	-0.76282
O	1.01304	-1.30174	0.81023
O	0.55122	0.22639	-1.01688
H	-0.88313	-0.15687	-0.42579
O	1.95259	1.00863	0.79401
H	2.87105	0.90910	1.07670
N	-1.84672	-0.38229	-0.02832
C	-1.82075	0.03664	1.40596
C	-2.03170	-1.85260	-0.17742
C	-2.82964	0.41464	-0.81611
H	-1.20545	-2.34437	0.33209

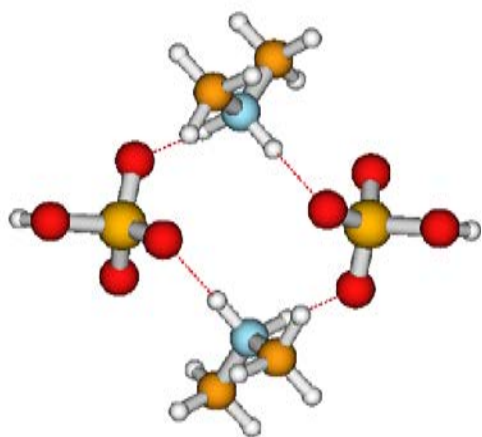
H	-2.00478	-2.10339	-1.23726
H	-2.99095	-2.14523	0.25225
H	-1.03497	-0.52760	1.90308
H	-2.79617	-0.15766	1.85505
H	-1.58219	1.09811	1.42500
H	-3.83562	0.22959	-0.43637
H	-2.76594	0.11532	-1.86172
H	-2.56347	1.46594	-0.71537
O	-0.57133	2.65670	-0.14110
H	0.01812	3.05817	0.50496
H	0.00235	2.00834	-0.58576



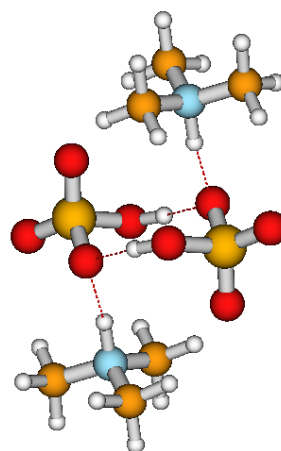
S	1.72033	0.00016	0.12841
O	1.86827	-1.22534	-0.65379
O	0.54608	-0.00073	1.01500
O	1.86625	1.22579	-0.65396
H	-0.98997	-0.00046	0.54143
O	2.93178	0.00126	1.22288
H	3.76136	0.00057	0.72570
N	-2.02610	-0.00043	0.33336
C	-2.57602	1.24402	0.94511
C	-2.57587	-1.24534	0.94432
C	-2.16470	-0.00001	-1.15695
H	-2.38512	-1.21924	2.01665
H	-2.06254	-2.09354	0.49203
H	-3.64997	-1.29180	0.75698
H	-2.38489	1.21744	2.01736
H	-3.65019	1.29028	0.75816
H	-2.06309	2.09261	0.49307
H	-3.22612	0.00001	-1.41190
H	-1.67565	-0.89977	-1.52898
H	-1.67576	0.90000	-1.52854

O	-0.46211	2.73532	-0.92496
H	-0.27688	3.38910	-1.60453
H	0.39376	2.28564	-0.77292
O	-0.46009	-2.73507	-0.92496
H	0.39573	-2.28540	-0.77261
H	-0.27518	-3.38689	-1.60649

a)



b)



c)

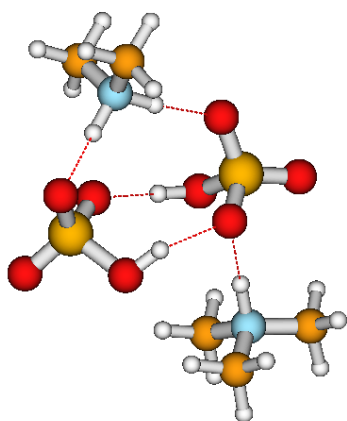


Figure S1. Most stable conformers of the clusters a) A_2D_2 , b) A_2T_2 and c) $A_2D_1T_1$.