Supplementary information for the article "Amines are likely to enhance neutral and ion-induced sulfuric acid - water nucleation in the atmosphere more effectively than ammonia" by Theo Kurtén, Ville Loukonen, Hanna Vehkamäki and Markku Kulmala.

Table S1. Electronic energies, enthalpies and entropies of all studied free molecules and clusters. DZ and TZ are shorthand for aug-cc-pV(D+d)Z and aug-cc-pV(T+d)Z, respectively. The single-point energies are computed at the RI-MP2/aug-cc-pV(D+d)Z geometries. Enthalpies and entropies are computed using the rigid rotor and harmonic oscillator approximations.

Species	E_0, RI-MP2/TZ (optimized) /Hartree	E_0, RI-MP2/DZ (optimized) /Hartree	E_0, RI-MP2/TZ single-point /Hartree	E_0, RI-CC2/TZ single-point /Hartree	H (T=298K) /kcal/mol	S (T=298K) /cal/molK
H_2SO_4	-699.4462	-699.1111	-699.4439	-699.4667	28.12	74.79
HSO_4^-	-698.9416	-698.6079	-698.9393	-698.9639	20.22	76.12
NH_3	-56.4605	-56.4049	-56.4604	-56.4620	23.96	49.77
CH_3NH_2	-95.6671	-95.5736	-95.6667	-95.6698	43.15	61.16
$(CH_3)_2NH$	-134.8811	-134.7496	-134.8805	-134.8851	61.64	68.48
$(CH_3)_3N$	-174.1009	-173.9317	-174.1000	-174.1067	79.69	72.13
$(CH_2CH_3)NH_2$		-134.7636	-134.8941	-134.8987	61.76	68.57
$(CH_2CH_3)_2NH$		-213.1285	-213.3338	-213.3415	98.93	83.19
$(CH_2CH_3)_3N$		-291.4977	-291.7769	-291.7885	135.89	95.72
$(CH_2CH_3)NH(CH_3)$		-173.9379	-174.1060	-174.1123	80.27	76.07
H_2SO_4•NH_3	-755.9340	-755.5430	-755.9315	-755.9564	53.39	92.96
HSO_4^-•NH_3	-755.4190	-755.0300	-755.4165	-755.4433	45.96	85.32
H_2SO_4•CH_3NH_2	-795.1483	-794.7196	-795.1455	-795.1729	73.24	99.34
HSO_4^-•CH_3NH_2	-794.6243	-794.1985	-794.6216	-794.6498	64.81	104.14
H_2SO_4•$(CH_3)_2NH$	-834.3690	-833.9033	-834.3659	-834.3952	92.24	106.13
HSO_4^-•$(CH_3)_2NH$	-833.8444	-833.3800	-833.8415	-833.8718	83.38	104.44
H_2SO_4•$(CH_3)_3N$	-873.5911	-873.0885	-873.5878	-873.6187	110.28	110.85
HSO_4^-•$(CH_3)_3N$	-873.0617	-872.5605	-873.0586	-873.0910	101.45	108.79
H_2SO_4•$(CH_2CH_3)NH_2$		-833.9127	-834.3754	-834.4044	91.96	105.14
HSO_4^-•$(CH_2CH_3)NH_2$		-833.3908	-833.8509	-833.8807	83.35	110.87
H_2SO_4•$(CH_2CH_3)_2NH$		-912.2875	-912.8240	-912.8563	129.52	120.33
HSO_4^-•$(CH_2CH_3)_2NH$		-911.7611	-912.2962	-912.3299	120.12	114.21
H_2SO_4•$(CH_2CH_3)_3N$		-990.6615	-991.2703	-991.3064	166.64	129.47

$HSO_4^-•(CH_2CH_3)_3N$		-990.1305	-990.7382	-990.7760	157.55	127.04
$H_2SO_4•(CH_2CH_3)NH(CH_3)$		-873.0939	-873.5935	-873.6243	110.93	114.08
$HSO_4^-•(CH_2CH_3)NH(CH_3)$		-872.5698	-873.0681	-873.1002	102.03	112.66
$(H_2SO_4)_2$		-1393.2509	-1398.9180	-1398.96437	57.51	113.18
$(H_2SO_4)_2•NH_3$		-1454.7012	-1455.4240	-1455.4728	84.03	119.86
$(H_2SO_4)_2•(CH_3)_2NH$		-1533.0681	-1533.8646	-1533.9167	122.16	136.08
$H_2SO_4•HSO_4^-$		-1397.7941	-1398.4611	-1398.5088	49.24	103.72
$H_2SO_4•HSO_4^-•NH_3$		-1454.2202	-1454.9405	-1454.9916	75.80	114.83
$H_2SO_4•HSO_4^-•(CH_3)_2NH$		-1532.5851	-1533.3784	-1533.4331	114.04	129.42

Table S2. The cartesian co-ordinates (in Ångström) of some free molecules and clusters, optimized at the RI-MP2/aug-cc-pV(T+d)Z level.

H_2SO_4

S	-4.37963E-10	-8.03323E-10	0.134855266
O	-0.568967938	1.122207128	0.800181228
O	0.568967925	-1.122207141	0.80018122
O	-1.077121981	-0.603824098	-0.863674457
O	1.077121995	0.603824111	-0.863674433
H	-1.670283031	0.113014369	-1.137083632
H	1.670283048	-0.113014352	-1.13708361

HSO_4^-

S	0.129844095	0.011094375	-1.36142E-05
O	0.489699009	-0.7006051	-1.222211016
O	0.406754022	1.434900007	-0.000214174
O	-1.535638005	0.002749593	0.000168998
O	0.489979134	-0.700309897	1.222271178
H	-1.762073414	-0.936001731	0.000195213

NH_3

N	0.0	0.0	0.068443035
H	-0.468166131	0.810887525	-0.31702698
H	-0.468166131	-0.810887525	-0.31702698
H	0.936332262	0.0	-0.31702698

CH_3NH_2

N	-0.071610434	-5.92535E-05	0.720880431
C	0.01378973	-7.37879E-05	-0.740505641
H	0.402441966	-0.809741552	1.100186281
H	0.402520143	0.80976624	1.099775353

H	1.031101655	-0.014339656	-1.142341172
H	-0.515597806	-0.868884674	-1.126550965
H	-0.489691878	0.884902296	-1.124390344

$(CH_3)_2NH$

N	8.36735E-05	-0.556266911	-0.085402604
C	-1.202414018	0.257350789	0.016007099
C	1.202356743	0.257411332	0.015978053
H	-0.000168567	-1.245485293	0.656055453
H	-1.253210014	0.921954916	-0.846694239
H	-2.083683519	-0.381156999	0.000409517
H	-1.234646246	0.879890618	0.920906327
H	1.255758885	0.918315185	-0.849394034
H	1.232099487	0.883918781	0.918253116
H	2.083369754	-0.381577514	0.006073346

$(CH_3)_3N$

N	-0.378892165	-2.74291E-06	-3.96442E-05
C	0.093569632	-1.213422559	-0.642651281
H	1.195040442	-1.265028328	-0.669868719
H	-0.277413318	-1.255998833	-1.666036106
H	-0.277570659	-2.083853032	-0.102874659
C	0.093566199	0.050130348	1.372158691
H	1.19503171	0.052212463	1.430404625
H	-0.277549274	-0.81483675	1.920660469
H	-0.277474489	0.952842592	1.856086484
C	0.093570351	1.163293426	-0.729474295
H	1.195040837	1.212753101	-0.760427931
H	-0.277548877	2.070751268	-0.254556401
H	-0.27743491	1.131181156	-1.753231476

$H_2SO_4 \bullet NH_3$

S	-0.532921208	-0.05136411	0.109702775
O	0.459412442	-0.858961007	-0.760350893
O	0.146358844	0.470019835	1.258648058
O	-0.830913636	1.23822494	-0.789497864
O	-1.743969366	-0.799793015	0.216298479
H	1.430719682	-0.536808853	-0.552982787
H	-1.527212329	0.997922493	-1.418817341
N	2.808496681	-0.002954947	-0.049699366
H	3.252360246	0.702719454	-0.624182582
H	3.501063299	-0.709639306	0.164505001
H	2.524315681	0.43522307	0.821315603

$HSO_4^- \bullet NH_3$

S	0.525527736	-0.100166545	3.08349E-05
O	-0.071739022	1.428111145	-0.000418075
O	-0.014592831	-0.708353892	1.219044593

O	-0.014579382	-0.709096542	-1.218614884
O	1.956726976	0.123126335	-5.74657E-05
H	-1.041327475	1.317334554	0.000314177
N	-2.666125839	0.052256082	-1.33865E-05
H	-2.219061174	-0.392123768	-0.799234776
H	-3.646527564	-0.1960176	-0.000164922
H	-2.2191837	-0.392583592	0.79901816

$H_2SO_4 \bullet CH_3NH_2$

S	-0.808879117	0.018105136	-0.114959475
O	-1.581388762	0.040152788	-1.328149909
O	-1.866482882	-0.043476422	1.101712606
O	0.024864755	-1.200747224	0.041292383
O	-0.030479282	1.217446668	0.199320036
N	2.231562375	-0.055204229	0.656533898
C	3.06896006	0.042272396	-0.5577753
H	-2.648582332	-0.498043057	0.758609929
H	1.432071592	-0.758617255	0.499104834
H	1.645994736	0.792241788	0.763941489
H	3.575442424	-0.903094595	-0.722455145
H	3.793941703	0.842667534	-0.449611689
H	2.405824395	0.252644479	-1.390840131
H	2.762997294	-0.252654816	1.496553662

$HSO_4^- \bullet CH_3NH_2$

S	-0.776017225	-0.000268727	-0.066007734
O	-0.20263825	-1.219407496	0.501342622
O	-0.951686861	-0.005298657	-1.503729262
O	-2.344063855	0.003090188	0.465079045
O	-0.200193154	1.221760653	0.492490406
N	2.671789416	-0.000420677	0.766824439
C	2.959733541	0.000307167	-0.671581162
H	-2.269575207	0.006298942	1.428127266
H	2.048168656	0.784369541	0.939039924
H	3.553443999	-0.879321705	-0.924038548
H	3.55546501	0.87890493	-0.922866584
H	2.063763114	0.001744734	-1.299812893
H	2.045643793	-0.783559255	0.937593554

$H_2SO_4 \bullet (CH_3)_2NH$

S	-1.159238974	0.003307583	0.113519475
N	1.993211784	-0.00281808	0.010670206
C	2.864673518	0.019485431	1.195813429
C	2.701987352	-0.022890044	-1.278813004
H	1.287806624	0.776405858	0.038603607
O	-0.321689793	1.212905105	0.097082649
O	-1.807345533	0.009951517	-1.36877999
O	-2.264971395	0.007779296	1.034091875
O	-0.321730802	-1.21085631	0.156549653

H	-2.709701208	-0.322615491	-1.265853207
H	2.238698701	0.032325837	2.083329192
H	3.491811526	-0.868431134	1.199418511
H	3.487942879	0.909646389	1.169387058
H	3.324216308	0.864485667	-1.362555353
H	3.322131641	-0.91382794	-1.3364531
H	1.963947158	-0.034182367	-2.075814708
H	1.290588959	-0.783252343	0.066185426

$HSO_4^-\bullet(CH_3)_2NH$

S	-1.243481896	0.085223212	-0.003166453
N	2.035712123	-0.102483396	0.124699471
C	3.218010781	0.067877471	0.945016144
C	2.333608148	-0.02243734	-1.297432392
H	1.336315799	0.609733411	0.35478899
O	-0.499691292	1.186776912	0.631629709
O	-1.017712796	0.023049629	-1.445787519
O	-2.623169012	-0.041573718	0.419025344
O	-0.551206635	-1.267597981	0.599607014
H	2.936801017	0.085065111	1.997373523
H	3.900725264	-0.770648975	0.787785638
H	3.771149345	0.992511089	0.718139954
H	2.888864874	0.890290826	-1.562042266
H	2.942559049	-0.880538168	-1.592623775
H	1.395216073	-0.040459418	-1.849421892
H	0.41399862	-1.137417914	0.467760787

$H_2SO_4\bullet(CH_3)_3N$

S	-1.373446662	-0.019215492	0.11757438
O	-0.375876398	-1.127972951	0.144710857
O	-0.699239471	1.266086717	0.176763595
O	-1.962241592	-0.05007948	-1.392251155
O	-2.494854612	-0.245521158	0.990584466
H	0.945602618	-0.484510147	0.067562567
H	-2.726522999	-0.642729207	-1.370575425
N	1.950620266	-0.060911952	0.002863026
C	2.884577325	-1.2012813	-0.045830934
H	3.906745025	-0.832885835	-0.120128519
H	2.64305892	-1.813038788	-0.911008533
H	2.763714068	-1.790439855	0.85933811
C	2.168739474	0.774683404	1.202097568
H	3.171638952	1.198731361	1.164559659
H	2.059365281	0.148775617	2.084109754
H	1.409695152	1.550877081	1.210004065
C	2.01030273	0.747542275	-1.233138753
H	3.010836241	1.165425274	-1.339382267
H	1.260355335	1.529066623	-1.156947906
H	1.780638191	0.103753007	-2.078507674

$HSO_4^-\bullet(CH_3)_3N$

S	-1.492096525	0.016442557	-0.02673788
O	-0.547812699	-1.218705646	0.476005102
O	-0.93373517	1.201361138	0.639518999
O	-1.322660508	0.060711902	-1.478742742
O	-2.809609355	-0.379895648	0.433292292
H	0.373908627	-0.942262973	0.255414179
N	2.030605195	-0.126202594	0.01066821
C	3.202421942	-0.946974352	-0.218643066
H	4.121690489	-0.339099678	-0.285009678
H	3.086459405	-1.498814268	-1.151478605
H	3.319542943	-1.660218228	0.5978898
C	2.144545882	0.600431595	1.267999847
H	3.010329103	1.284399073	1.256135442
H	2.271803673	-0.109275418	2.08627147
H	1.224126429	1.161627448	1.424474694
C	1.836854944	0.811782793	-1.089812731
H	2.711042114	1.477717359	-1.193117108
H	0.938307754	1.395384454	-0.901383156
H	1.693712401	0.258995476	-2.017088658

Table S3. The cartesian co-ordinates (in Ångström) of all studied free molecules and clusters, optimized at the RI-MP2/aug-cc-pV(D+d)Z level.

H_2SO_4

S	-2.24259E-08	-4.70672E-09	0.143445565
O	-1.270524664	-0.157153882	0.808885506
O	1.270524561	0.157153121	0.808885796
O	0.213486251	-1.239950934	-0.879555067
O	-0.213486112	1.239951645	-0.879554144
H	-0.671098631	-1.538452059	-1.159815317
H	0.671098795	1.538452995	-1.159814077

HSO_4^-

S	0.137354939	0.016663893	-2.70049E-06
O	0.524234542	-0.693310386	-1.241247904
O	0.356192078	1.472067698	-4.34274E-05
O	-1.569867292	-0.055275205	3.12178E-05
O	0.524284357	-0.693246921	1.241262951
H	-1.74781673	-1.010006151	4.08781E-05

NH_3

N	1.44846E-06	-4.88542E-10	0.069281128
H	-0.471233378	0.816394648	-0.320906238
H	-0.471419881	-0.816286967	-0.32090624
H	0.942633132	-0.000107674	-0.32091457

CH_3NH_2

N	-0.073043953	-3.83151E-06	0.725464577
C	0.014135377	-3.52934E-06	-0.744572852
H	0.41182673	-0.813548663	1.104085527
H	0.41186932	0.813572112	1.103965897
H	1.041723076	-0.000439007	-1.152763503
H	-0.509799805	-0.886083652	-1.132007244
H	-0.509043928	0.886594508	-1.131836963

$(CH_3)_2NH$

N	3.01657E-06	-0.560720165	-0.086557439
C	-1.209761919	0.259095774	0.01612531
C	1.209768967	0.259088609	0.016126681
H	2.01104E-05	-1.243050125	0.671854936
H	-1.265443253	0.923367069	-0.861008335
H	-2.099129386	-0.388186002	0.008141516
H	-1.240487762	0.894722378	0.926237191
H	1.263624399	0.925686622	-0.859352072
H	1.241996	0.89235179	0.927826831
H	2.099293988	-0.387930128	0.004777241

$(CH_3)_3N$

N	-0.383474568	-2.09532E-05	3.00217E-07
C	0.094844519	-0.700627176	-1.19027838
H	1.20779397	-0.731177138	-1.242189771
H	-0.280844974	-0.195732602	-2.093444883
H	-0.280863539	-1.735331035	-1.187317755
C	0.094844578	-0.680472577	1.201914775
H	1.207794017	-0.710169794	1.254319054
H	-0.28088906	-1.715069143	1.216403069
H	-0.280819409	-0.160413981	2.096446975
C	0.094837462	1.381110115	-0.011636581
H	1.207786005	1.441303196	-0.012147488
H	-0.280838991	1.910903332	0.877164654
H	-0.280844017	1.895854856	-0.909235805

$(CH_2CH_3)NH_2$

N	-0.300413859	-1.185720976	-0.068722556
H	-0.917014184	-1.226804372	0.744946109
C	0.579292238	-0.007319268	0.035129103
C	-0.260331823	1.267423498	-0.017308894
H	1.20262914	-0.001892056	0.950774873
H	1.266884612	-0.032811002	-0.825740463
H	-0.847213845	1.298717838	-0.947567248
H	0.379757596	2.16232323	0.032998697
H	-0.962267118	1.305806004	0.832605549
H	0.250970451	-2.044247479	-0.045401149

$(CH_2CH_3)_2NH$

N	0.471699	-0.237708	-0.074508
H	0.245204	0.068751	0.871135
C	1.339339	-1.41318	-0.022194
H	0.733438	-2.255876	0.33002
C	2.521898	-1.250171	0.922769
C	1.056876	0.868116	-0.828427
C	0.065088	2.020033	-0.896823
H	1.687662	-1.685046	-1.02541
H	3.07699	-2.191474	0.99186
H	3.217184	-0.480696	0.574126
H	2.188894	-0.983574	1.931364
H	1.978186	1.224419	-0.356001
H	1.29713	0.548291	-1.848635
H	-0.865082	1.713614	-1.387358
H	0.490567	2.849908	-1.470283
H	-0.180484	2.392881	0.103377

$(CH_2CH_3)_3N$

N	-0.417801766	0.178940441	0.022027555
C	-0.69761322	-0.896932963	-0.9456767
H	-1.274569271	-1.679737879	-0.42826736
C	0.519566868	-1.531412636	-1.641182691
C	0.137356412	1.365081828	-0.646232948
C	0.00991896	2.633466732	0.201530513
H	-1.3720272	-0.4680323	-1.705981648
H	0.17864704	-2.296058717	-2.357889348
H	1.104722127	-0.785066295	-2.200707329
H	1.190561491	-2.025891409	-0.921510717
H	1.203540782	1.217222458	-0.930390365
H	-0.429379408	1.505638156	-1.582387427
H	-1.036612842	2.778242916	0.509638758
H	0.329780546	3.508594002	-0.386613758
H	0.639392389	2.596486736	1.102898167
C	0.45652759	-0.253848851	1.121730465
H	1.486497959	-0.477294624	0.760464621
H	0.547246606	0.592583222	1.819178219
C	-0.095688984	-1.456870221	1.887872505
H	-0.072683355	-2.379730777	1.288869394
H	-1.134709674	-1.266634984	2.198979529
H	0.512200358	-1.6324528	2.789291123

$(CH_2CH_3)NH(CH_3)$

N	-0.609035706	0.705966176	0.260892428
H	-0.657461596	0.646862176	1.279534915
C	-0.607997086	-0.653506931	-0.29616116
H	-1.561581442	-1.126481115	-0.007873124
C	0.558869158	-1.560206301	0.125566466
C	0.565376315	1.496006715	-0.121783708

H	-0.622741211	-0.553684415	-1.39579012
H	0.434096342	-2.568536969	-0.301944505
H	1.528506721	-1.169667894	-0.219040803
H	0.597335833	-1.659459407	1.22338313
H	1.537463022	1.081639541	0.209952101
H	0.587931779	1.580344957	-1.220370609
H	0.46787213	2.511231582	0.290834163

$H_2SO_4 \bullet NH_3$

S	-0.544920931	-0.049595288	0.117777419
O	0.455773125	-0.934478823	-0.724452353
O	0.127727175	0.474701091	1.292661935
O	-0.743613524	1.265624539	-0.832760919
O	-1.807329274	-0.753249857	0.179397434
H	1.420196047	-0.595581586	-0.52946658
H	-1.405281913	1.025694139	-1.505856513
N	2.821262624	-0.010312745	-0.050707022
H	3.27610731	0.660456109	-0.669600961
H	3.52442563	-0.697482318	0.219768849
H	2.543626163	0.493002708	0.794861077

$HSO_4^- \bullet NH_3$

S	0.530143713	-0.105991791	2.39792E-05
O	-0.081726041	1.459119846	-0.000276272
O	-0.019153228	-0.721013001	1.238173506
O	-0.019235396	-0.721539268	-1.237834048
O	1.980686044	0.12943111	-9.89769E-05
H	-1.054213036	1.331557223	0.000176977
N	-2.67755082	0.052389331	-2.35871E-05
H	-2.234235801	-0.405603416	-0.802648239
H	-3.666293737	-0.194221592	-0.000416773
H	-2.234918505	-0.405504509	0.803021104

$H_2SO_4 \bullet CH_3NH_2$

S	-0.80017316	0.017733779	-0.123406419
O	-1.627343668	-0.064001978	-1.321532977
O	-1.836999059	0.053972276	1.16026476
O	0.045401864	-1.217735006	0.107533911
O	0.00415168	1.242390654	0.084898501
N	2.258957998	-0.072788288	0.691243541
C	2.974121531	0.059533172	-0.60672872
H	-2.611515878	-0.466123026	0.885411636
H	1.381056979	-0.713667907	0.545529244
H	1.80158295	0.817156257	0.935102422
H	3.348214133	-0.926304566	-0.906905011
H	3.804089617	0.770603937	-0.514533293
H	2.242343056	0.421122844	-1.33808371
H	2.860169852	-0.397008969	1.448831338

$HSO_4^-•CH_3NH_2$

S	-0.756244443	3.89095E-05	-0.057563311
O	-0.215877567	-1.239759081	0.551871127
O	-0.84917638	0.000398994	-1.5240975
O	-2.395032061	-0.000343462	0.380130793
O	-0.216270016	1.23967771	0.552521626
N	2.687500433	-5.01707E-05	0.768212298
C	2.887479033	-1.19505E-05	-0.694390728
H	-2.36964263	-0.000506963	1.351045659
H	2.067000582	0.788905407	0.973906051
H	3.473081508	-0.888582077	-0.982858276
H	3.474139583	0.887915209	-0.982699831
H	1.947221742	0.000578048	-1.274359012
H	2.066012721	-0.788297644	0.973678982

$H_2SO_4•(CH_3)_2NH$

S	-1.161325724	0.010924453	0.16497786
N	1.960336882	0.017132041	0.103414138
C	3.157641565	0.004634726	0.970275422
C	2.23483119	-0.038599813	-1.354806045
H	1.322831253	0.8291707	0.287361512
O	-0.366485176	1.258061196	0.33621552
O	-1.337911378	-0.015094939	-1.494347362
O	-2.506486437	-0.004259918	0.722127227
O	-0.341803247	-1.208784302	0.467054366
H	-2.107121422	-0.585569826	-1.664720709
H	2.835390987	0.048623894	2.018112334
H	3.722443304	-0.920329991	0.793110421
H	3.786529149	0.874040546	0.736173395
H	2.833638096	0.834826541	-1.645308442
H	2.781222366	-0.963434383	-1.582650487
H	1.26875475	-0.029309497	-1.875904705
H	1.264523538	-0.743811242	0.338051705

$HSO_4^-•(CH_3)_2NH$

S	-1.249118639	0.090332204	-0.005316347
N	2.041084653	-0.105588897	0.127566165
C	3.234774992	0.075571398	0.944251301
C	2.330003345	-0.02868385	-1.305505572
H	1.341071602	0.615173455	0.357592799
O	-0.491358874	1.210274915	0.634004561
O	-1.016336625	0.014081835	-1.468163298
O	-2.647407916	-0.040079439	0.425918915
O	-0.543756425	-1.292046932	0.622289169
H	2.955248687	0.09599438	2.008918787
H	3.927107081	-0.770018774	0.785997235
H	3.790212575	1.010960321	0.709309235
H	2.886210903	0.893843624	-1.582794462
H	2.94511711	-0.8956116	-1.605049085

H	1.376900293	-0.05215213	-1.853058658
H	0.423984715	-1.152545934	0.482734525

$H_2SO_4 \bullet (CH_3)_3N$

S	-1.380594673	-0.048549147	0.138252939
O	-0.392998462	-1.196668367	0.125886374
O	-0.732513428	1.18999318	0.600979096
O	-1.624343717	0.27724885	-1.478714967
O	-2.684046362	-0.412959236	0.679587935
H	0.936830147	-0.515332821	0.097069812
H	-2.351806991	-0.307855174	-1.75130591
N	1.927319336	-0.063296283	0.008278443
C	2.870312688	-1.173215795	-0.275427309
H	3.888118462	-0.771981009	-0.392032768
H	2.552972113	-1.675401851	-1.198779777
H	2.837684911	-1.885886221	0.559226559
C	2.243391015	0.619520638	1.289956905
H	3.242553131	1.076054892	1.219851406
H	2.223436648	-0.126101778	2.095957425
H	1.469025258	1.374800769	1.467432642
C	1.85885412	0.901543358	-1.122982169
H	2.856625289	1.336046697	-1.287573836
H	1.123308535	1.672528603	-0.865284008
H	1.52219112	0.362110896	-2.018149212

$HSO_4^- \bullet (CH_3)_3N$

S	-1.49839759	0.019499199	-0.030050655
O	-0.536495484	-1.231807736	0.524504356
O	-0.945916848	1.235947496	0.633397161
O	-1.298472742	0.034459702	-1.500902875
O	-2.838044461	-0.385667051	0.424875263
H	0.384191273	-0.950068733	0.285818775
N	2.033417716	-0.123452334	0.0121424
C	3.204972937	-0.958680056	-0.222295279
H	4.14014668	-0.355236864	-0.30007594
H	3.074856492	-1.521214255	-1.160240683
H	3.321981345	-1.676490743	0.605582372
C	2.160607992	0.613193727	1.272537959
H	3.040830878	1.297294679	1.257742217
H	2.284513186	-0.101994868	2.101699678
H	1.236244984	1.187259893	1.431212993
C	1.833863811	0.814141072	-1.099093703
H	2.721564523	1.477896173	-1.224035449
H	0.93508159	1.412858317	-0.899583825
H	1.66785407	0.249298415	-2.028383098

$H_2SO_4 \bullet (CH_2CH_3)NH_2$

S	-1.128646232	-0.092669476	0.016678441
O	-0.345803027	-0.560432487	-1.182362486

O	-0.376665345	-0.343793602	1.273051043
O	-1.082822795	1.563128271	-0.086221249
O	-2.539101274	-0.458916994	-0.008559257
H	1.076761944	-1.007860038	-0.662546988
H	-1.906702417	1.812011677	-0.538962979
N	1.864406236	-1.151095696	0.055629439
H	1.293831953	-1.001135508	0.914578479
C	2.935472802	-0.118640188	-0.087497221
C	2.322685266	1.274250395	0.023640231
H	3.685187152	-0.296330618	0.697247627
H	3.409933022	-0.274958143	-1.066875262
H	1.56270596	1.433149984	-0.754318619
H	3.116190401	2.026886254	-0.091851519
H	1.839369803	1.41480331	1.001506601
H	2.218724149	-2.107940339	0.023532086

HSO_4^-•$(CH_2CH_3)NH_2$

S	-1.039739065	0.038735704	-0.033771222
O	-0.853926196	0.929801235	1.133960411
O	-0.373545502	-1.280175756	0.123483811
O	-2.694511591	-0.328141884	-0.025124971
O	-0.887989646	0.66600753	-1.353693106
H	-2.836902474	-0.711473471	0.855849357
N	2.362288419	-0.300259316	1.232417231
H	1.502126057	-0.839199558	1.06978359
C	2.519872413	0.573991158	0.050611888
C	2.722137359	-0.284637475	-1.197148652
H	1.647235227	1.233708768	-0.108039275
H	3.404934231	1.216177486	0.213409468
H	3.600312782	-0.94051524	-1.074563223
H	2.86599736	0.347524859	-2.08927212
H	1.828636246	-0.907179402	-1.36003728
H	2.11947354	0.291705822	2.030431037

H_2SO_4•$(CH_2CH_3)_2NH$

S	-1.577885942	-0.291591332	-0.027721466
O	-0.955006665	0.050576435	-1.328026084
O	-0.529816542	-0.639716028	0.999780794
O	-2.160136056	1.183014755	0.471352284
O	-2.722139541	-1.195146863	-0.037153856
H	0.962243326	0.241598523	-1.18531738
H	-2.922888673	0.978165624	1.038679761
N	1.580050918	0.071197233	-0.371413971
H	0.826900479	-0.233344829	0.333874746
C	2.500157883	-1.069790585	-0.634819113
H	1.882070686	-1.857586498	-1.089655305
C	3.145614994	-1.568910952	0.654509482
C	2.204151144	1.34698365	0.075023215
C	1.137785284	2.438012568	0.14110165
H	3.249624536	-0.742207894	-1.372164698

H	3.726289425	-2.47867853	0.442916799
H	3.831717879	-0.826503259	1.087291082
H	2.371059308	-1.819526304	1.395815321
H	2.652256756	1.168921208	1.0625119
H	3.008239117	1.597764048	-0.635240141
H	0.711803884	2.632115883	-0.854809024
H	1.58664127	3.36856771	0.517813778
H	0.316162737	2.141488523	0.809466587

$HSO_4^-\bullet(CH_2CH_3)_2NH$

S	-1.698515806	-0.114609937	0.125934062
O	-1.113993738	-0.05407144	-1.443409574
O	-0.778842498	-1.068253534	0.820448659
O	-1.562509447	1.26802463	0.643579615
O	-3.071382262	-0.598994306	-0.06625389
H	-0.155695512	0.155843941	-1.337791897
N	1.58297681	0.076324966	-0.382168022
H	0.864100031	-0.137295829	0.326886279
C	2.299910989	-1.177598258	-0.635480015
H	1.563466044	-1.885299	-1.050260659
C	2.959938547	-1.810249904	0.60029113
C	2.422626249	1.180357367	0.088519609
C	1.602550626	2.47188227	0.110271879
H	3.058696712	-0.988085099	-1.417933964
H	3.417839396	-2.781094176	0.34304305
H	3.749599231	-1.16473298	1.017741668
H	2.196960924	-1.981207129	1.376877092
H	2.84695807	0.996039279	1.098354636
H	3.279451058	1.276553312	-0.605553218
H	1.303579699	2.747561756	-0.912908437
H	2.185220933	3.300465495	0.547922665
H	0.679471557	2.32452899	0.693033179

$H_2SO_4\bullet(CH_2CH_3)_3N$

S	-1.919981476	-0.255134043	-0.134883994
O	-0.835278071	-0.254852533	-1.187437677
O	-1.333508881	-0.242644194	1.215031803
O	-2.585948317	1.267991796	-0.246657447
O	-3.007074376	-1.186792542	-0.421296281
H	0.465893379	0.025682184	-0.416364148
H	-3.306843494	1.184775899	-0.893750579
N	1.482629718	0.186708505	-0.083158567
C	2.299277341	-0.450503171	-1.170130551
H	1.925619568	-1.477568501	-1.277843798
C	3.804208369	-0.425124683	-0.922245821
C	1.697205879	1.670706845	-0.02631252
C	0.62285997	2.397731178	0.779059273
H	2.034901117	0.087881775	-2.092506251
H	4.306663223	-0.892552454	-1.782366366
H	4.192875359	0.599439229	-0.827886799

H	4.083111548	-0.995388081	-0.024154052
H	2.701919039	1.846963193	0.388944691
H	1.685222497	2.018604535	-1.07075223
H	-0.380297362	2.191552607	0.382716395
H	0.81558584	3.478809311	0.701299453
H	0.643912483	2.12757772	1.84319642
C	1.65690826	-0.459707648	1.258995765
H	2.668962887	-0.211613514	1.617802205
H	0.911939829	0.007141251	1.912383688
C	1.409356605	-1.964222253	1.211876189
H	2.207104287	-2.511043983	0.687838743
H	0.439589096	-2.17236282	0.737607636
H	1.36448345	-2.340725227	2.244399929

$HSO_4^-\bullet(CH_2CH_3)_3N$

S	-2.097804727	-0.090864666	-0.094828984
O	-0.924136877	-0.635284652	-1.155852149
O	-1.508123547	-0.33682346	1.2509294
O	-2.253501997	1.354488892	-0.399198336
O	-3.257391164	-0.930143638	-0.438233584
H	-0.078665924	-0.246664997	-0.800391226
N	1.555265927	0.185356067	-0.131288446
C	2.429218189	-0.474612918	-1.114804377
H	2.046642791	-1.4958408	-1.271423757
C	3.92827415	-0.531328543	-0.771246386
C	1.806243741	1.634250534	-0.068991829
C	0.741428617	2.393086823	0.728453865
H	2.288378428	0.060652288	-2.069793698
H	4.475445264	-1.031133186	-1.588077465
H	4.357682173	0.474875377	-0.64445102
H	4.108242724	-1.102187177	0.153309162
H	2.815404049	1.846851857	0.354180348
H	1.80428771	1.998857163	-1.11147288
H	-0.271332501	2.130902731	0.383223702
H	0.900155531	3.476170852	0.590061504
H	0.811787589	2.183090169	1.806013813
C	1.601384186	-0.431586928	1.207206437
H	2.578168707	-0.223341128	1.703327641
H	0.803523838	0.039297837	1.795952624
C	1.315127883	-1.933608636	1.174792891
H	2.12967362	-2.513887239	0.710405168
H	0.372173083	-2.1122826	0.637511272
H	1.190313911	-2.295430582	2.207794847

$H_2SO_4\bullet(CH_2CH_3)NH(CH_3)$

S	-1.506724036	-0.21669663	0.006509878
O	-0.840345148	-0.092118203	-1.328580533
O	-0.539838361	-0.627309587	1.064928548
O	-1.807689008	1.360252028	0.465098337
O	-2.795853777	-0.89380825	-0.008177982

H	0.845631769	0.107828012	-1.03989043
H	-2.658764031	1.591401642	0.05471787
N	1.57640018	0.195795245	-0.288614511
H	1.010638084	-0.246587158	0.483636609
C	2.81318873	-0.56925158	-0.597342919
H	2.483275485	-1.563238911	-0.932990785
C	3.729080736	-0.682850557	0.617334098
C	1.746806289	1.637385025	0.025808637
H	3.313909485	-0.068143447	-1.44017241
H	4.580549644	-1.334226593	0.371978645
H	4.131825603	0.29348843	0.923143848
H	3.190988989	-1.128918173	1.468308869
H	2.318656857	1.751738028	0.95420868
H	2.268788285	2.128984655	-0.806229109
H	0.743468263	2.064623167	0.153291616

HSO_4^-•$(CH_2CH_3)NH(CH_3)$

S	-1.453258029	-0.056119202	0.090237206
O	-1.029290694	-1.350699766	-0.494803883
O	-0.674474553	0.292318387	1.318628344
O	-0.995524519	1.105599442	-1.027768028
O	-2.903097786	0.155180923	0.188684717
H	-0.012646504	1.145769077	-0.969374233
N	1.770217555	0.703842462	-0.196432638
H	1.082804319	0.584499787	0.564538677
C	2.103232642	-0.638540103	-0.708173074
H	1.248775656	-0.986745867	-1.307632552
C	2.371144001	-1.677109296	0.389733424
C	2.93144981	1.432613596	0.309920858
H	2.978397983	-0.535231119	-1.377358123
H	2.611007764	-2.658752495	-0.054124969
H	3.21139368	-1.384506495	1.041838433
H	1.460619323	-1.787244809	0.999175813
H	3.511228984	0.890416546	1.086473499
H	3.617607106	1.658198227	-0.524964771
H	2.597731742	2.387970581	0.744271739

$(H_2SO_4)_2$

S	0.115672178	-0.019671862	-2.058354202
O	-0.76372483	-1.169442604	-1.415297239
O	1.14373742	0.411183626	-1.115689951
O	-0.89759737	1.240300779	-2.096283553
O	0.443918735	-0.439153637	-3.395187346
H	-0.915384707	-0.949151283	-0.452947849
H	-1.524391181	1.097009004	-2.829750138
S	-0.115671241	0.019671933	2.058353388
O	0.897599108	-1.240299908	2.09629248
O	-1.143734724	-0.411187721	1.115688803
O	0.763722984	1.169440863	1.415290797
O	-0.443919937	0.439160712	3.395184103

H	1.524339358	-1.097041802	2.829811233
H	0.915384724	0.949148323	0.452942908

$(H_2SO_4)_2 \bullet NH_3$

S	1.839922539	-0.291866675	-0.038511143
O	2.50331349	0.860452397	-0.707153365
O	1.08967168	0.17995142	1.169054166
O	3.032143348	-1.258669461	0.487017401
O	1.072943173	-1.186477009	-0.914604143
H	1.459099841	2.128279123	-0.368145688
H	3.675438667	-0.699171133	0.95682441
S	-2.093213366	-0.094000465	-0.021372891
O	-1.470668095	-0.351835084	1.417752935
O	-3.521528045	-0.191265907	0.089054437
O	-1.590274092	-1.319204055	-0.889500072
O	-1.489381947	1.136955036	-0.570874747
H	-0.474541434	-0.216635261	1.365371116
H	-0.5924077	-1.278288422	-0.959480871
N	0.636115982	2.703679068	-0.042401756
H	-0.22291331	2.114453285	-0.182345447
H	0.558265978	3.581303968	-0.555661366
H	0.747900617	2.885219543	0.955907446

$(H_2SO_4)_2 \bullet (CH_3)_2NH$

S	-2.215747504	0.009386325	0.149536765
O	-1.42007792	0.537347431	-0.975267082
O	-3.64119596	-0.114650272	0.017611397
O	-1.631137902	-1.416651271	0.539265361
O	-1.926794295	0.907621204	1.423706112
H	-0.624609752	-1.350178532	0.552629411
H	-0.934754172	0.965092763	1.558953629
N	0.940912324	0.058876582	-2.223870088
H	0.04366948	0.062466555	-1.692568614
H	1.658971652	0.287825966	-1.499974654
C	0.883696513	1.146404759	-3.233084554
H	0.062699931	0.941776351	-3.932266531
H	1.839734999	1.189393593	-3.770894491
H	0.700805082	2.092551004	-2.709287318
C	1.187589309	-1.291604737	-2.788345463
H	0.373810704	-1.541582153	-3.481790168
H	1.217036782	-2.004845978	-1.956578458
H	2.147716014	-1.28698261	-3.320743736
S	1.628414035	0.068678583	1.00034758
O	0.967370332	-1.149925104	0.432352046
O	0.706291702	0.891897376	1.814754378
O	2.414353677	0.78609747	-0.020649073
O	2.774493769	-0.456744392	2.026887978
H	2.325449894	-0.688502233	2.859211618

$H_2SO_4 \bullet HSO_4^-$

S	-0.001527875	1.880857942	-0.081337096
O	1.26090122	1.374187076	0.73185257
O	-1.237547878	1.366793851	0.765997989
O	-0.003839227	3.326382094	-0.02241875
O	-0.017552686	1.213964338	-1.391721829
H	1.273180283	0.347364874	0.683984761
H	-1.260585809	0.34024267	0.699538787
S	-0.000201646	-1.869809077	0.09278671
O	1.232167753	-1.192943411	0.61479477
O	-1.240155385	-1.195302914	0.600429445
O	0.000833496	-3.319561061	0.213729571
O	0.00797117	-1.599968144	-1.520749372
H	-0.001679845	-0.61926816	-1.619399178

$H_2SO_4 \bullet HSO_4^- \bullet NH_3$

S	2.065875038	0.070859817	0.193025379
O	3.343801751	0.223749339	0.877474329
O	1.102875756	1.207957506	0.317511926
S	-2.046994467	-0.042509392	0.197299301
O	-2.104476177	0.906995893	-0.970453978
O	-3.348765336	-0.408272203	0.74281839
O	-1.141261252	-1.193911454	-0.146803728
N	-0.120474324	-0.014114458	-2.462239385
H	-0.859203534	0.489879106	-1.8770602
O	1.353980221	-1.192211865	0.930745376
H	0.419325407	-1.240996934	0.586810463
H	-0.461427634	-0.972471032	-2.548735708
H	-0.018663435	0.41148279	-3.381039352
O	-1.306564222	0.757904813	1.391383557
H	-0.389259998	0.978937197	1.058864116
O	2.198367906	-0.321811718	-1.258008421
H	0.827847297	-0.061433943	-1.955222306

$H_2SO_4 \bullet HSO_4^- \bullet (CH_3)_2NH$

S	-2.053295115	0.010044273	0.580985185
O	-3.326359372	0.297871783	1.231523547
O	-1.130559028	1.181413996	0.397721933
O	-1.286582341	-0.993834958	1.600217782
O	-2.172973275	-0.735011536	-0.72134309
H	-0.371962499	-1.131801557	1.22459252
S	2.053461914	-0.009996649	0.580786104
O	2.171186538	0.733794692	-0.722219157
O	3.327161928	-0.296523874	1.23066783
O	1.131247508	-1.182192061	0.399602963
O	1.287088778	0.99423179	1.60028773
H	0.372787615	1.1331411	1.224419194
N	-0.002102885	-0.000822675	-2.087545861
C	-0.481836925	1.146610861	-2.881941971

H	0.341039599	1.535522684	-3.499128638
H	-0.827280854	1.913196155	-2.17698982
H	-1.316559235	0.825107877	-3.521273017
C	0.483364933	-1.14571921	-2.882359083
H	1.32236718	-0.821504529	-3.51465528
H	-0.334971627	-1.532938432	-3.506601765
H	0.824556913	-1.914244387	-2.177478576
H	0.794103176	0.319424219	-1.466991924
H	-0.801717663	-0.322640412	-1.471240592