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Supplement of

Electrical charging changes the composition of sulfuric acid–ammonia/ dimethylamine clusters

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Supplementary Material

Clusters included in the study

	1 base	2 bases	3 bases	4 bases
HSO_4^-	NH_3 DMA			
$(\text{H}_2\text{SO}_4)\cdot\text{HSO}_4^-$	NH_3 DMA	DMA		
$(\text{H}_2\text{SO}_4)_2\cdot\text{HSO}_4^-$	NH_3 DMA	NH_3 DMA	DMA	
$(\text{H}_2\text{SO}_4)_3\cdot\text{HSO}_4^-$	NH_3 DMA	NH_3 DMA	NH_3 DMA	DMA
$(\text{H}_2\text{SO}_4)_4\cdot\text{HSO}_4^-$	NH_3	NH_3	NH_3	NH_3

Table S-1a. Schematic diagram of the negatively charged clusters included in this study. NH_3 indicates ammonia-containing and DMA indicates DMA-containing clusters.

	$\text{H}^+ + 1$ base	$\text{H}^+ + 2$ bases	$\text{H}^+ + 3$ bases	$\text{H}^+ + 4$ bases	$\text{H}^+ + 5$ bases
0 acids	NH_3 DMA	NH_3 DMA	NH_3 DMA		
H_2SO_4	NH_3 DMA	NH_3 DMA	NH_3 DMA		
$(\text{H}_2\text{SO}_4)_2$	NH_3 DMA	NH_3 DMA	NH_3 DMA	NH_3 DMA	
$(\text{H}_2\text{SO}_4)_3$			NH_3 DMA	NH_3 DMA	NH_3
$(\text{H}_2\text{SO}_4)_4$			NH_3 DMA	NH_3 DMA	NH_3 DMA
$(\text{H}_2\text{SO}_4)_5$					NH_3

Table S-1b. Schematic diagram of the positively charged clusters included in this study. NH_3 indicates ammonia-containing and DMA indicates DMA-containing clusters.

Dipole moments and polarizabilities used to estimate the collision rate of charged clusters.

	Dipole moment (D)	Polarizability (\AA^3)
H ₂ SO ₄	2.96 ^a	6.2 ^b
(H ₂ SO ₄) ₂	0.002	9.061
(H ₂ SO ₄) ₃	3.692	13.710
(H ₂ SO ₄) ₄	3.252	18.759
NH ₃	1.47 ^c	2.81 ^c
H ₂ SO ₄ ·NH ₃	5.259	6.073
(H ₂ SO ₄) ₂ ·NH ₃	9.309	10.733
(H ₂ SO ₄) ₃ ·NH ₃	4.580	15.482
(H ₂ SO ₄) ₄ ·NH ₃	8.006	20.171
(H ₂ SO ₄) ₅ ·NH ₃	4.103	24.822
(NH ₃) ₂	0.000	3.106
H ₂ SO ₄ ·(NH ₃) ₂	3.990	7.826
(H ₂ SO ₄) ₂ ·(NH ₃) ₂	6.762	12.455
(H ₂ SO ₄) ₃ ·(NH ₃) ₂	10.065	17.121
(H ₂ SO ₄) ₄ ·(NH ₃) ₂	9.769	21.828
(H ₂ SO ₄) ₅ ·(NH ₃) ₂	8.476	26.755
(NH ₃) ₃	0.000	4.964
H ₂ SO ₄ ·(NH ₃) ₃	7.430	9.633
(H ₂ SO ₄) ₂ ·(NH ₃) ₃	4.006	14.184
(H ₂ SO ₄) ₃ ·(NH ₃) ₃	7.700	18.719
(H ₂ SO ₄) ₄ ·(NH ₃) ₃	7.163	23.637
(H ₂ SO ₄) ₅ ·(NH ₃) ₃	5.099	28.112
(NH ₃) ₄	0.000	6.797
H ₂ SO ₄ ·(NH ₃) ₄	5.798	11.458
(H ₂ SO ₄) ₂ ·(NH ₃) ₄	4.208	15.980
(H ₂ SO ₄) ₃ ·(NH ₃) ₄	2.150	20.630
(H ₂ SO ₄) ₄ ·(NH ₃) ₄	4.011	25.383
(H ₂ SO ₄) ₅ ·(NH ₃) ₄	8.191	30.007
(CH ₃) ₂ NH	1.01 ^c	6.37 ^c
H ₂ SO ₄ ·(CH ₃) ₂ NH	8.755	9.367
(H ₂ SO ₄) ₂ ·(CH ₃) ₂ NH	7.842	13.941
(H ₂ SO ₄) ₃ ·(CH ₃) ₂ NH	9.113	18.640
(H ₂ SO ₄) ₄ ·(CH ₃) ₂ NH	7.938	23.277
((CH ₃) ₂ NH) ₂	0.000	10.170
H ₂ SO ₄ ·((CH ₃) ₂ NH) ₂	6.823	14.733
(H ₂ SO ₄) ₂ ·((CH ₃) ₂ NH) ₂	5.843	18.876
(H ₂ SO ₄) ₃ ·((CH ₃) ₂ NH) ₂	7.606	23.345
(H ₂ SO ₄) ₄ ·((CH ₃) ₂ NH) ₂	0.411	28.419
((CH ₃) ₂ NH) ₃	0.012	15.451
H ₂ SO ₄ ·((CH ₃) ₂ NH) ₃	5.909	19.762
(H ₂ SO ₄) ₂ ·((CH ₃) ₂ NH) ₃	7.030	24.141
(H ₂ SO ₄) ₃ ·((CH ₃) ₂ NH) ₃	6.338	28.669
(H ₂ SO ₄) ₄ ·((CH ₃) ₂ NH) ₃	8.378	33.305
((CH ₃) ₂ NH) ₄	0.005	20.512
H ₂ SO ₄ ·((CH ₃) ₂ NH) ₄	1.415	25.246
(H ₂ SO ₄) ₂ ·((CH ₃) ₂ NH) ₄	9.154	29.324
(H ₂ SO ₄) ₃ ·((CH ₃) ₂ NH) ₄	5.046	33.774
(H ₂ SO ₄) ₄ ·((CH ₃) ₂ NH) ₄	4.802	38.239

a: from Sedo et al. (2008)

b: from Nadykto and Yu (2003)

c: from CRC Handbook of Chemistry and Physics (2010)

Table S-2. Dipole moments and polarizabilities of all studied clusters at 298 K. For molecules we used experimental values, except for the sulfuric acid polarizability, for which only a theoretical value is available, and for clusters we used values calculated for the minimum-free energy clusters (at the corresponding temperature) with the Gaussian09 program (Frisch et al. 2009) using the B3LYP hybrid functional (*Becke et al. 1993*) and a CBSB7 basis set (Montgomery et al. 1999).

xyz of the most stable clusters.

Negatively charged pure sulfuric acid clusters

$\text{H}_2\text{SO}_4\cdot\text{HSO}_4^-$

13

S	1.885090	0.081878	0.000971
O	1.376614	-0.738685	-1.240795
O	1.367591	-0.739236	1.236822
O	3.313294	0.025501	0.004899
O	1.226273	1.378451	-0.001615
H	0.354647	-0.696966	-1.276651
H	0.343513	-0.690978	1.273184
S	-1.874131	-0.097435	-0.000002
O	-1.193334	-0.604079	-1.216305
O	-1.194390	-0.591910	1.222778
O	-3.303785	-0.239057	0.000822
O	-1.620295	1.509093	-0.007310
H	-0.649250	1.636231	-0.006401

$(\text{H}_2\text{SO}_4)_2\cdot\text{HSO}_4^-$

20

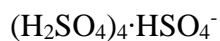
S	-3.402718	-0.665977	0.086856
O	-4.624573	-1.397614	0.092963
O	-2.988707	0.066657	1.270349
O	-3.456725	0.339533	-1.128678
O	-2.249106	-1.670606	-0.305472
H	-2.632864	0.914614	-1.117660
H	-1.363831	-1.202866	-0.248619
O	-0.603486	1.515140	1.418243
H	-1.464583	1.058408	1.544134
S	-0.134979	1.224480	-0.086018
O	0.006473	-0.260567	-0.184989
O	-1.202932	1.706251	-0.967354
O	1.127465	1.924658	-0.209801
S	3.589058	-0.609430	0.091543
O	2.421418	-1.372519	-0.673792
O	3.565649	0.833031	-0.579684
H	1.539203	-0.997576	-0.414300
H	2.707291	1.283850	-0.370979
O	4.811005	-1.222723	-0.321655
O	3.242645	-0.491440	1.481036

$(\text{H}_2\text{SO}_4)_3\cdot\text{HSO}_4^-$

27

S	-4.582865	-0.289105	-0.316335
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O	-5.969527	-0.167189	-0.607113
O	-3.749086	-1.195850	-1.084679
O	-4.450593	-0.666233	1.212967
O	-3.950038	1.158097	-0.402773
H	-3.489368	-0.825418	1.428803
H	-2.959424	1.096306	-0.312238
S	-0.903022	-0.530220	0.498288
O	-1.030533	-1.571147	-0.704069
O	-1.811365	-0.956269	1.558279
O	0.518094	-0.587895	0.839132
O	-1.295787	0.797087	-0.054376
H	-1.975930	-1.587092	-0.978495
S	3.744335	-1.650886	-0.079470
O	3.799361	-0.741894	-1.382224
O	4.737322	-2.658963	-0.256511
H	3.280562	0.085034	-1.236922
O	3.716406	-0.796272	1.078477
O	2.335835	-2.380476	-0.200774
H	1.633307	-1.801634	0.178442
S	1.885307	2.464999	-0.089611
O	2.626689	3.675780	0.003791
O	2.227943	1.461370	-1.077931
O	1.899185	1.788112	1.342094
O	0.374959	2.866592	-0.299455
H	1.595242	0.853229	1.274036
H	-0.215397	2.064150	-0.278237



34

S	3.088858	-3.088795	-0.257419
S	-5.022801	-0.887229	0.084916
S	-1.247783	-0.820358	0.182592
S	0.086804	3.614295	-0.381960
O	-1.836774	-1.784508	-0.733723
O	0.218749	-0.794573	0.162562
O	-1.840020	0.536830	0.008899
O	-6.443335	-0.887168	0.043808
O	-4.323401	-1.186704	1.321350
O	2.741622	-2.788769	1.104960
O	3.395051	-4.409323	-0.699055
O	1.359803	4.104771	0.117541
O	-0.923826	4.549454	-0.745200
O	-1.589887	-1.263994	1.673141
O	-4.531543	0.526155	-0.431270
O	-4.518481	-1.889935	-1.029171
O	4.340190	-2.198450	-0.684177
O	1.931428	-2.533636	-1.202954
O	-0.400534	2.605840	0.721048
O	0.331914	2.692721	-1.642744
H	-3.552685	0.616213	-0.286714
H	-3.527402	-1.954928	-0.984791
H	-2.572366	-1.300260	1.744363
H	1.300464	-1.979768	-0.690383
H	4.322032	-1.333588	-0.218468
H	1.097808	2.088608	-1.462554
H	-1.015493	1.889981	0.380694
S	3.070234	1.112923	0.390987
O	3.388850	2.551740	0.909798

O	2.037923	0.617778	1.459943
O	4.290298	0.360702	0.486105
O	2.421424	1.172478	-0.905540
H	2.628925	3.164450	0.690063
H	1.318141	0.064655	1.039388

Negatively charged ammonia-sulfuric acid clusters

HSO₄⁻·NH₃

10

S	0.609055	-0.107742	0.000002
O	-0.023887	1.435959	0.000052
O	0.074161	-0.724944	1.223621
O	0.073177	-0.725259	-1.223090
O	2.040100	0.135704	-0.000608
H	-0.992113	1.307460	0.000214
N	-2.596280	0.057730	0.000008
H	-2.150145	-0.393704	-0.798525
H	-3.584509	-0.172057	-0.001427
H	-2.152552	-0.393627	0.799862

H₂SO₄·HSO₄⁻·NH₃

17

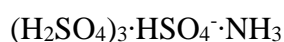
S	-2.104870	-0.234201	-0.078803
O	-3.404161	-0.854328	-0.089359
O	-1.167455	-0.657974	-1.134823
S	2.074151	-0.238942	0.038329
O	2.100363	0.879453	-0.942730
O	3.372956	-0.728493	0.423075
O	1.174472	0.125680	1.170172
N	0.162154	2.421402	-0.006605
H	0.886325	1.884725	-0.576835
O	-1.431331	-0.702040	1.317508
H	-0.467850	-0.475363	1.298201
H	0.468806	2.259298	0.953280
H	0.146557	3.410622	-0.231564
O	1.360092	-1.470948	-0.700496
H	0.422325	-1.213450	-0.908185
O	-2.164833	1.257688	-0.011374
H	-0.820565	1.962339	-0.096860

(H₂SO₄)₂·HSO₄⁻·NH₃

24

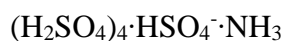
S	0.000023	1.513211	0.154400
O	0.000007	0.094345	-0.476417
O	1.230499	2.192324	-0.300333
O	-1.230490	2.192319	-0.300248
O	0.000098	1.327896	1.630784
N	-0.000194	-1.249107	2.000910
H	0.000152	-1.631407	2.941174
H	-0.860003	-1.513810	1.495009
H	0.859276	-1.513823	1.494484

H	-0.000151	-0.171144	1.999482
S	3.236392	-0.672189	-0.240863
S	-3.236380	-0.672171	-0.240947
O	2.610220	-1.279322	0.926807
O	-4.485804	-1.207253	-0.681714
O	-2.610260	-1.279974	0.926412
O	4.485780	-1.207546	-0.681395
O	3.434079	0.863768	0.017348
O	-3.433954	0.863677	0.018097
O	-2.219790	-0.725995	-1.435728
H	2.563421	1.394848	-0.065286
H	-2.563384	1.394811	-0.065016
H	-1.305322	-0.389230	-1.115598
O	2.219789	-0.726573	-1.435650
H	1.305433	-0.389449	-1.115753



31

N	-0.138314	-1.211746	-0.331102
H	-0.987024	-1.756403	-0.133500
H	0.673739	-1.768688	-0.622593
H	-0.399976	-0.506549	-1.058572
S	-1.966329	1.530177	-0.714776
O	-1.777175	0.885015	0.609943
O	-1.115270	0.907403	-1.734211
H	3.318653	3.305903	1.514824
S	2.226845	1.781744	0.510444
O	3.076643	2.403100	1.762493
O	3.189918	1.585973	-0.579022
O	1.759942	0.508982	1.087575
O	1.192544	2.755275	0.215381
H	0.124365	-0.648596	0.484653
O	-3.376593	1.644355	-1.081814
H	-4.295213	0.260941	-0.845097
S	3.770012	-1.910173	-0.320729
O	4.533825	-0.661925	-0.901553
O	3.480734	-1.509505	1.184251
O	4.688909	-2.998836	-0.301066
O	2.502044	-2.051300	-1.009511
H	3.985884	0.177428	-0.832165
H	2.831064	-0.748444	1.218283
S	-4.125155	-1.484831	0.419536
O	-3.719985	-0.514861	1.592872
O	-5.105193	-2.394750	0.914552
O	-4.854476	-0.538711	-0.614509
O	-2.913993	-2.005913	-0.188270
H	-2.962190	0.082614	1.284936
O	-1.472282	3.037617	-0.546986
H	-0.523794	2.997988	-0.285657



38

S	-0.398361	-0.279180	-0.992393
O	-1.882325	-0.085948	-1.094249
O	-0.083074	-1.715667	-1.235082
O	0.289966	0.603805	-1.975354

O	0.045361	0.099631	0.382282
N	-1.586634	0.724761	2.362541
H	-0.893755	0.839446	3.112831
H	-2.007597	1.615704	2.089316
H	-2.277008	-0.000157	2.565865
H	-1.036766	0.393844	1.525653
S	-2.939299	-2.833434	0.687852
S	2.221409	0.913493	2.757383
S	3.381065	-1.164331	-1.668340
S	-1.899327	3.331183	-0.924860
O	1.018936	0.781329	3.552485
O	3.353459	1.570712	3.326369
O	-2.595525	-1.828828	1.672469
O	3.240374	-0.571738	-0.353597
O	-2.403523	4.641656	-1.162052
O	-1.747281	2.848470	0.431518
O	4.663561	-1.558021	-2.142623
O	1.904293	1.641413	1.395450
O	2.577648	-0.562764	2.295053
O	-3.834929	-3.886519	1.029955
O	-1.611825	-3.512427	0.155125
O	2.772473	-0.160452	-2.725423
O	2.438979	-2.427599	-1.762370
O	-0.504366	3.235845	-1.672062
O	-2.807795	2.310689	-1.720039
H	1.223308	1.119329	0.881304
H	2.962445	-0.575116	1.386854
H	-1.016194	-2.855315	-0.295596
H	1.883444	0.181629	-2.430325
H	1.500032	-2.189479	-1.516761
H	-0.180977	2.299425	-1.747563
H	-2.515211	1.376740	-1.509386
O	-3.515071	-2.104282	-0.590347
H	-2.937755	-1.317491	-0.814328



28

S	3.127914	-1.027915	0.067332
O	2.787773	-0.606030	1.443234
O	3.087422	0.334199	-0.825501
O	4.462341	-1.535899	-0.111367
H	2.295796	0.862091	-0.578605
S	-2.711515	-1.269772	0.009879
O	-3.055582	0.127075	0.223859
O	-4.130351	-2.033761	0.319086
O	-2.378049	-1.623274	-1.377431
H	-3.953825	-2.978363	0.216328
S	-0.273991	2.545442	-0.030039
O	0.564672	1.422081	-0.560176
O	-0.494004	2.347660	1.413277
O	-1.708768	2.346646	-0.741687
O	0.166167	3.850516	-0.440443
O	2.058403	-1.891898	-0.492396
N	0.222846	-0.191407	2.162152
N	0.202111	-0.793559	-2.048821
H	-2.179934	1.581123	-0.339749
H	0.950995	-1.314920	-1.503071
H	0.420891	-0.783559	-3.040016

H	-0.736849	-1.206365	-1.877601
H	0.208247	0.178904	-1.663852
H	1.211277	-0.400995	1.845820
H	-0.455844	-0.834092	1.711707
H	-0.028277	0.796067	1.902643
H	0.160612	-0.300663	3.170305
O	-1.753313	-1.820882	0.975550



35

N	-1.735395	2.146441	0.405698
H	-0.909969	2.472780	-0.159418
H	-2.625573	2.132945	-0.110115
H	-1.814970	2.720009	1.241075
N	1.768085	-1.297360	1.675908
H	2.727479	-1.500277	1.244280
H	1.752410	-1.599542	2.645613
H	1.576918	-0.275062	1.621808
S	1.533841	1.733421	-0.132778
O	0.652157	2.724460	-0.755459
O	1.635771	0.469284	-0.926212
O	1.128409	1.418629	1.251635
H	0.140709	-0.206706	-1.251569
S	-1.379821	-1.455650	-0.310346
O	-0.812928	-0.465624	-1.419229
O	-2.554074	-2.058049	-0.933680
O	-0.322420	-2.379538	0.067754
O	-1.778959	-0.578586	0.843882
H	-1.558398	1.157417	0.683744
H	1.030135	-1.788347	1.141169
O	2.956137	2.380598	-0.126172
H	3.638832	1.697309	0.226038
S	-5.048564	0.178716	0.072126
O	-4.995201	-1.077922	-0.870422
O	-4.331231	-0.311089	1.395884
O	-6.416129	0.423053	0.389296
O	-4.252957	1.244421	-0.510944
H	-4.054744	-1.420910	-0.968438
H	-3.353482	-0.477363	1.222483
S	4.858812	-0.646932	0.019295
O	4.270633	-0.403051	-1.470719
O	6.266144	-0.857387	-0.171452
O	4.493231	0.576109	0.785498
O	4.120500	-1.810205	0.564530
H	3.320885	-0.169539	-1.394181



42

S	2.688606	0.187607	1.430394
O	3.140529	0.298179	-0.031330
O	3.314099	-1.022178	2.016408
O	3.043640	1.423468	2.129571
O	1.191171	-0.003882	1.402338
N	0.289159	0.352874	-1.147663
H	-0.738391	0.302892	-1.229478
H	0.668697	1.249132	-1.478628

H	0.730666	-0.449212	-1.605828
H	0.559740	0.291748	-0.136192
S	2.936508	-2.920665	-0.869461
S	-2.807238	-1.374613	-0.328614
S	-5.706033	0.985338	0.190763
S	2.660667	3.611922	-0.623851
O	-2.565757	-0.011565	-0.872629
O	-1.680604	-2.269184	-0.547005
O	1.646278	-2.332180	-1.181573
O	-4.970816	0.512780	1.350764
O	2.967216	4.883738	-1.189381
O	1.436676	2.937947	-1.017804
O	-6.797488	1.882384	0.350442
O	-4.114053	-1.895863	-0.720730
O	-2.819271	-1.208132	1.279687
O	3.333710	-4.124433	-1.521844
O	2.949255	-3.199891	0.708041
O	-6.240555	-0.273116	-0.604013
O	-4.679588	1.653268	-0.807989
O	2.675472	3.779508	0.944599
O	3.874362	2.644589	-0.904882
H	-3.550470	-0.587427	1.502700
H	3.170172	-2.342754	1.229164
H	-5.512340	-0.952269	-0.670596
H	-3.849619	1.100564	-0.856494
H	2.749211	2.894570	1.412606
H	3.644577	1.717702	-0.579966
O	4.054516	-1.846129	-1.048875
H	3.735201	-0.947964	-0.659244
N	0.173153	-2.481229	1.500145
H	-0.282759	-2.765073	2.363112
H	0.966181	-3.092569	1.277250
H	0.559023	-1.495644	1.588938
H	-0.516569	-2.493095	0.717240



39

S	1.922290	2.518457	-0.167115
O	2.268476	2.360138	1.248310
O	3.277413	3.113572	-0.866386
O	1.727308	1.258309	-0.892224
H	3.685512	3.701832	-0.217607
S	-3.792065	-0.186795	-1.256514
O	-2.523239	0.218022	-1.936585
O	-3.593979	-1.732983	-0.853922
O	-3.913664	0.557778	0.022576
H	-2.935713	-1.791154	-0.120435
S	-1.425009	-0.616543	1.994557
O	-0.760218	-0.980550	3.235221
O	-1.631704	-1.739633	1.052770
O	-0.740437	0.512064	1.320956
O	-2.877600	-0.103839	2.406723
H	-3.370244	0.107351	1.564576
O	0.869313	3.501779	-0.418149
N	1.962830	-0.230198	2.395817
N	-1.672350	2.347528	-0.429710
N	-0.034016	-1.050659	-1.256218
H	-1.455511	1.721274	0.379978

H	-1.961887	1.694904	-1.194756
H	-2.457661	2.948086	-0.197081
H	-0.811671	2.885783	-0.634580
H	-0.840116	-0.826959	-1.854046
H	-0.387619	-1.525124	-0.413083
H	0.728006	-1.612705	-1.698859
H	0.399784	-0.169842	-0.951336
H	1.038550	-0.437729	2.811180
H	1.971350	0.734279	2.013570
H	2.145545	-0.919936	1.600190
H	2.692300	-0.326160	3.096804
O	-4.952795	-0.159656	-2.102131
S	3.150272	-2.075722	-0.734465
O	3.881067	-0.618395	-0.796329
O	4.236285	-3.005701	-0.581348
O	2.234202	-1.986488	0.438322
O	2.359438	-2.186657	-1.972203
H	3.197376	0.056977	-0.981957



46

S	1.425019	0.237449	0.343385
O	2.738616	0.872906	-0.008580
O	1.649751	-0.958267	1.195797
O	0.578604	1.230460	1.090070
O	0.700476	-0.163004	-0.898662
N	-1.466054	1.587543	-1.280367
H	-2.204812	1.570275	-0.538088
H	-0.893109	2.444618	-1.225134
H	-1.921985	1.518761	-2.186891
H	-0.818004	0.782025	-1.162891
S	4.604459	-2.177395	0.091981
S	-2.426363	-2.597702	-0.542434
S	-4.661331	0.665472	0.393273
S	1.531680	4.180372	-0.368881
O	-2.487335	-1.298852	-1.245742
O	-1.978023	-3.703736	-1.367635
O	3.587163	-2.786751	-0.747147
O	-3.373245	1.373186	0.715877
O	1.791460	5.580321	-0.391080
O	0.498365	3.633950	-1.231322
O	-5.828869	1.482575	0.554938
O	-1.628934	-2.479057	0.710240
O	5.872993	-2.812973	0.219186
O	4.009131	-1.976105	1.536503
O	-4.668332	-0.643938	1.073652
O	-4.562082	0.357179	-1.188536
O	1.212959	3.765232	1.118545
O	2.891236	3.444361	-0.679164
H	3.085024	-1.571744	1.469903
H	-3.865663	-0.339907	-1.308876
H	0.963153	2.789957	1.156375
H	2.821877	2.462167	-0.491622
O	4.867413	-0.704752	-0.412794
H	4.055168	-0.127682	-0.315099
N	0.755438	-2.904988	-0.788230
H	0.333946	-2.950932	0.146340
H	1.748544	-3.172664	-0.779157

H	0.705582	-1.890609	-1.040734
H	0.154208	-3.461391	-1.402501
N	-1.643101	-0.159118	2.157094
H	-1.654754	-1.079453	1.648142
H	-0.738032	0.314836	1.980750
H	-1.795022	-0.307054	3.150328
H	-2.404202	0.438614	1.748584
O	-3.918583	-2.946026	-0.107146
H	-4.293433	-2.148686	0.357901



50

S	1.791947	0.312436	0.657576
O	3.099840	0.937929	0.271608
O	2.021131	-0.905236	1.474567
O	0.970364	1.297686	1.431354
O	1.033578	-0.064542	-0.577414
N	-1.234392	1.159936	-1.530995
H	-1.853924	1.598710	-0.829858
H	-1.020221	1.825173	-2.269883
H	-1.723107	0.295841	-1.841370
H	-0.329422	0.868439	-1.098133
S	4.906759	-2.149355	0.162052
S	-2.312003	-2.473296	-0.910038
S	-4.539735	1.097800	0.615894
S	1.616244	4.028929	-0.650881
O	-2.754188	-1.123278	-1.438286
O	-1.423397	-3.132478	-1.881548
O	3.866225	-2.656657	-0.711523
O	-3.160883	1.647734	0.509404
O	1.741823	5.423447	-0.921296
O	0.694274	3.220922	-1.419364
O	-5.588693	2.072889	0.727410
O	-1.590270	-2.264944	0.388133
O	6.162399	-2.822665	0.220651
O	4.336494	-2.061165	1.629405
O	-4.551409	0.030482	1.651798
O	-4.819186	0.333848	-0.780836
O	1.267379	3.872212	0.883497
O	3.065574	3.405870	-0.763632
H	3.431884	-1.608886	1.619300
H	-4.031731	-0.248105	-1.017995
H	1.122722	2.905773	1.111683
H	3.074736	2.459572	-0.438890
O	5.203619	-0.644033	-0.212480
H	4.397335	-0.063543	-0.083005
N	1.000986	-2.795961	-0.683937
H	0.704407	-2.990516	0.271164
H	1.939564	-3.161591	-0.861726
H	1.045320	-1.752501	-0.746806
H	0.231009	-3.123411	-1.308822
N	-1.480760	-0.042954	1.936806
H	-1.511295	-0.908166	1.326739
H	-0.537902	0.391628	1.921992
H	-1.756758	-0.287639	2.883183
H	-2.166929	0.638445	1.548128
O	-3.539961	-3.302988	-0.674028
N	-5.527842	-2.211519	0.488939

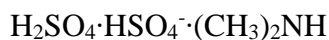
H	-6.119885	-1.807844	-0.234012
H	-4.644371	-2.700227	-0.001437
H	-5.190117	-1.405282	1.076051
H	-6.056345	-2.876864	1.045009

Negatively charged DMA-sulfuric acid clusters



16

S	1.395645	-0.001320	-0.092674
N	-1.955967	-0.125586	0.081676
C	-3.147999	-0.938360	-0.063589
C	-2.204891	1.309537	0.036356
H	-1.254217	-0.366278	-0.625464
O	0.615150	-0.565433	-1.214303
O	1.215531	1.446875	0.044165
O	2.763919	-0.475243	-0.000335
O	0.683504	-0.658752	1.261596
H	-2.869757	-1.995036	-0.098139
H	-3.813699	-0.795276	0.797056
H	-3.737273	-0.709721	-0.973029
H	-2.774977	1.625491	-0.857819
H	-2.777465	1.620887	0.919370
H	-1.242062	1.823264	0.040869
H	-0.276595	-0.509749	1.142617



23

S	2.067402	-0.674397	-0.004779
O	3.349483	-1.287511	-0.242497
O	1.169065	-0.579099	-1.181691
O	1.321448	-1.652628	1.035871
O	2.140075	0.653403	0.667340
H	0.394911	-1.319463	1.160862
S	-2.067389	-0.674336	0.004724
O	-2.140195	0.653376	-0.667476
O	-3.349385	-1.287522	0.242700
O	-1.168801	-0.579017	1.181464
O	-1.321596	-1.652670	-1.036009
H	-0.395123	-1.319515	-1.161196
N	0.000111	2.079293	-0.000091
C	0.467634	2.863600	-1.159497
H	-0.350288	3.468308	-1.555625
H	0.808946	2.155885	-1.913509
H	1.298692	3.505136	-0.861397
C	-0.467834	2.862376	1.159988
H	-1.299309	3.503640	0.862467
H	0.349752	3.467245	1.556565
H	-0.808668	2.153800	1.913402
H	-0.804804	1.453535	-0.307106
H	0.805343	1.453595	0.306505

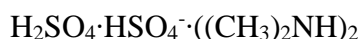


S	-3.688160	-0.064763	0.040689
O	-5.093232	-0.259215	0.274189
O	-2.786073	-0.483190	1.142546
O	-3.333365	-1.046920	-1.198112
O	-3.324033	1.303025	-0.413863
H	-2.357824	-1.034379	-1.316973
S	0.179332	-1.355944	0.003929
O	0.603856	-0.192880	0.854169
O	1.300004	-2.245220	-0.274652
O	-0.555583	-0.876942	-1.170719
O	-0.824189	-2.200499	0.883738
H	-1.641392	-1.627742	1.037744
N	-0.799253	2.003685	0.009532
C	-0.804591	3.043292	1.060922
H	0.219973	3.317276	1.315565
H	-1.309036	2.637903	1.937039
H	-1.347050	3.919392	0.704025
C	-0.140686	2.394061	-1.262269
H	0.919475	2.574236	-1.085356
H	-0.629020	3.282773	-1.664199
H	-0.242852	1.559436	-1.952392
H	-0.308182	1.157976	0.375865
H	-1.805173	1.703455	-0.179188
S	3.841181	0.242563	-0.052924
O	3.141220	0.212095	1.369036
O	3.797358	-1.275659	-0.507768
O	3.035721	1.037302	-0.948245
O	5.216882	0.564156	0.159001
H	2.158254	0.047872	1.242448
H	2.863057	-1.626210	-0.494877



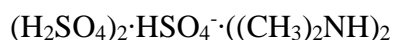
S	-1.511574	-3.269509	-0.589475
O	-1.989421	-4.500308	-1.127431
O	-1.271403	-2.267084	-1.777663
O	-2.317120	-2.593337	0.419318
H	-1.000474	-1.359293	-1.408074
S	0.336544	-0.001044	0.455115
O	-0.365071	-0.001111	1.733102
O	1.180258	1.223721	0.272339
O	-0.697076	-0.000143	-0.682590
O	1.179060	-1.226398	0.271570
N	-3.076644	0.003970	1.121689
C	-4.290463	0.001755	0.269249
H	-4.869255	-0.897772	0.473497
H	-3.972843	0.004012	-0.771630
H	-4.874361	0.897453	0.475935
C	-3.331834	0.002296	2.583927
H	-2.363658	0.003586	3.078374
H	-3.892735	-0.894375	2.846470
H	-3.896095	0.896414	2.848022
H	-2.505819	-0.824796	0.883766
H	-2.509355	0.835632	0.884547
O	-0.074062	-3.525366	-0.009536
H	0.411950	-2.656650	0.162847

S	-1.505551	3.271753	-0.589392
O	-2.311436	2.598866	0.421450
O	-1.980976	4.503342	-1.127650
O	-0.066450	3.523692	-0.012230
O	-1.270785	2.267479	-1.777108
H	0.417035	2.653330	0.160705
H	-0.999928	1.359644	-1.407619
S	4.527291	-0.002283	0.018705
O	4.184273	-0.000730	-1.376445
O	5.889780	-0.003405	0.448596
O	3.832294	-1.244471	0.729068
O	3.833534	1.239215	0.731554
H	2.868326	1.268137	0.497262
H	2.866938	-1.271779	0.495015



33

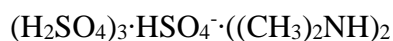
S	2.246270	-1.118055	-0.091347
O	3.479829	-1.637966	-0.632822
O	2.408002	0.070267	0.778271
O	1.425294	-0.597375	-1.387735
O	1.382531	-2.136000	0.550034
H	0.535121	-0.222903	-1.129665
S	-2.073537	1.035868	-0.179234
O	-2.559434	-0.065087	0.743831
O	-3.154741	1.548301	-1.006567
O	-0.954448	0.456491	-1.014034
O	-1.474325	2.129762	0.683135
N	-1.316693	-2.257056	0.384118
C	-1.700735	-3.187467	1.459114
H	-2.783965	-3.323120	1.456556
H	-1.397121	-2.757682	2.413531
H	-1.204751	-4.151586	1.325257
C	-1.656316	-2.715925	-0.978529
H	-2.733070	-2.882990	-1.044810
H	-1.115465	-3.635594	-1.213093
H	-1.374184	-1.922842	-1.668465
H	-1.822106	-1.275159	0.550239
H	-0.281642	-2.102320	0.435913
N	1.039369	2.378187	0.389745
H	1.508779	1.446672	0.491147
H	-0.059433	2.221422	0.523139
C	1.263895	2.889488	-0.977945
C	1.530364	3.260314	1.462208
H	1.006620	4.217184	1.417784
H	1.325079	2.785105	2.421330
H	2.606542	3.420320	1.362929
H	2.333982	2.990373	-1.173474
H	0.767752	3.855940	-1.086052
H	0.820501	2.178651	-1.672010



40

S	-3.332236	1.073716	-0.076425
O	-4.763740	1.153412	-0.224479
O	-2.653531	2.331232	0.293352

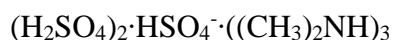
O	-3.106968	0.052539	1.163445
O	-2.629375	0.433924	-1.225157
H	-2.154787	0.074177	1.465602
S	0.381113	-1.023207	1.269494
O	-0.292459	-2.345827	1.184324
O	1.677492	-1.114239	1.973649
O	-0.509958	-0.007229	1.886332
O	0.642132	-0.549196	-0.176275
N	-1.995228	-2.152019	-0.860398
C	-1.263981	-2.639378	-2.049717
H	-1.046546	-3.702447	-1.936569
H	-0.331100	-2.082507	-2.112411
H	-1.864491	-2.474058	-2.945681
C	-3.277361	-2.833909	-0.579683
H	-3.096562	-3.893453	-0.392108
H	-3.951312	-2.712683	-1.428867
H	-3.716186	-2.364329	0.299088
H	-1.351825	-2.243372	-0.016673
H	-2.193092	-1.120680	-0.981549
N	0.025305	2.141933	-0.207528
H	-1.009554	2.220230	-0.052054
H	0.247761	1.117604	-0.174787
C	0.728032	2.823681	0.910304
C	0.371071	2.645237	-1.557101
H	1.431468	2.469514	-1.734439
H	-0.235427	2.103000	-2.281523
H	0.143237	3.710500	-1.617073
H	0.453034	3.879731	0.911235
H	1.801142	2.699177	0.778163
H	0.405595	2.345975	1.833168
S	3.914454	0.087782	-0.469953
O	5.213348	-0.068864	-1.050909
O	3.315513	1.409148	-0.444406
O	3.983783	-0.481650	0.995882
O	2.930373	-0.896247	-1.203586
H	1.985660	-0.793179	-0.800944
H	3.059683	-0.685060	1.372858



47

S	-1.916309	1.371320	-1.106524
O	-3.338913	1.542141	-1.390451
O	-1.700257	0.554131	0.137441
O	-1.365064	0.482382	-2.288015
O	-1.140170	2.609085	-1.050570
H	-0.333045	0.425780	-2.274523
S	1.825392	-0.821593	-1.474770
O	1.672358	-0.509857	0.020931
O	3.259870	-0.899255	-1.806980
O	1.177633	0.316277	-2.203202
O	1.116597	-2.093730	-1.751049
N	1.339592	2.207425	0.202521
C	1.354124	2.603732	1.632382
H	2.321804	2.335693	2.053076
H	0.557050	2.065386	2.143968
H	1.180944	3.677456	1.713965
C	2.352948	2.897306	-0.641950
H	3.340783	2.681235	-0.240805

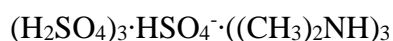
H	2.151083	3.969359	-0.634493
H	2.260737	2.497490	-1.649619
H	1.495335	1.168038	0.141963
H	0.399090	2.374305	-0.205856
N	-1.216683	-2.179646	-0.452526
H	-1.459474	-1.190359	-0.255826
H	-0.266459	-2.158473	-0.926095
C	-2.201841	-2.748321	-1.408307
C	-1.115099	-2.899753	0.840319
H	-0.832351	-3.935707	0.651782
H	-0.341337	-2.415350	1.434106
H	-2.076509	-2.850088	1.349447
H	-3.190219	-2.731738	-0.954433
H	-1.900844	-3.765886	-1.659436
H	-2.190934	-2.128574	-2.303096
S	-4.750959	-0.277860	1.327570
O	-5.790188	-0.378882	2.300023
O	-4.182759	-1.476234	0.748717
O	-3.577461	0.570003	1.968446
O	-5.289987	0.654649	0.171992
H	-4.555210	0.933076	-0.450285
H	-2.806617	0.596471	1.323935
S	4.750967	-0.240916	1.313912
O	5.803585	-0.544364	2.232153
O	5.219548	-0.717548	-0.111541
O	4.262957	1.122780	1.224956
H	4.448760	-0.749632	-0.770281
O	3.533660	-1.186468	1.641477
H	2.759516	-0.966829	1.010264



50

S	3.492747	-1.170698	1.020873
O	4.081151	-2.225228	1.807348
O	2.977450	-1.597150	-0.309518
O	2.182069	-0.715116	1.850579
O	4.322192	0.046560	0.866212
H	1.816842	0.137562	1.471163
S	0.134837	1.520730	-0.251374
O	0.792092	1.437089	-1.590063
O	-0.732886	2.721884	-0.145970
O	1.189867	1.528185	0.805461
O	-0.752528	0.304619	-0.051658
N	3.428782	1.446352	-1.254830
C	4.126871	0.826816	-2.400261
H	3.781757	1.277747	-3.332096
H	3.898098	-0.237646	-2.384235
H	5.203904	0.966240	-2.293552
C	3.694620	2.885106	-1.044824
H	3.373140	3.449386	-1.921131
H	4.759251	3.042808	-0.863879
H	3.114879	3.197150	-0.177802
H	2.375725	1.339210	-1.376821
H	3.709073	0.920370	-0.383936
N	0.282867	-2.172542	-0.290026
H	1.318807	-2.032241	-0.301406
H	-0.123467	-1.212686	-0.132803
C	-0.094664	-3.051258	0.846831

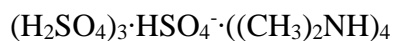
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H	-1.263175	-2.765299	-1.581567
H	0.091291	-1.901454	-2.359330
H	0.307525	-3.599425	-1.848777
H	0.327018	-4.045047	0.686830
H	-1.181715	-3.092996	0.898435
H	0.328341	-2.618970	1.752128
S	-3.908703	-1.187417	-0.535891
O	-4.162982	-0.357057	0.677946
O	-5.096983	-1.454101	-1.313312
O	-3.061895	-2.343499	-0.230785
O	-3.016618	-0.215088	-1.503340
H	-2.161242	-0.022090	-1.047213
N	-3.004773	1.960867	1.103950
C	-4.078540	2.959647	0.933208
C	-2.498954	1.821294	2.488263
H	-2.179160	2.217582	0.498474
H	-4.936827	2.680501	1.545281
H	-3.716177	3.948308	1.220052
H	-4.375682	2.967112	-0.114710
H	-2.094355	2.774337	2.830858
H	-3.308998	1.490666	3.139182
H	-1.707094	1.075339	2.474243
H	-3.387498	1.008361	0.811172



57

S	-2.115147	0.766225	1.210535
O	-3.514156	0.847209	1.682847
O	-1.730528	-0.666687	0.946791
O	-1.970187	1.512937	-0.101306
O	-1.165034	1.350591	2.195924
S	2.201823	1.105533	-1.068649
O	1.782220	-0.260066	-0.520549
O	3.591844	1.015191	-1.560442
O	2.089200	2.086605	0.055665
O	1.250818	1.469435	-2.154635
N	1.175808	-0.132844	2.169677
C	0.968556	-1.535879	2.610683
H	1.887027	-2.093185	2.431494
H	0.137446	-1.943715	2.039556
H	0.717491	-1.544309	3.672178
C	2.219796	0.596694	2.934611
H	3.152781	0.040921	2.866663
H	1.896577	0.696024	3.972040
H	2.348947	1.572969	2.472905
H	1.439182	-0.142359	1.155372
H	0.270128	0.390206	2.220748
N	-1.013401	-0.110205	-2.137473
H	-1.448287	0.275428	-1.271937
H	-0.083843	0.370471	-2.189400
C	-1.856020	0.306572	-3.285471
C	-0.834754	-1.580720	-2.022462
H	-0.338607	-1.946723	-2.922472
H	-0.212095	-1.771165	-1.153919
H	-1.814041	-2.038984	-1.904057
H	-2.845920	-0.129019	-3.164512
H	-1.391542	-0.028419	-4.213592

H	-1.928437	1.393305	-3.283560
S	-4.738971	-1.764912	-0.285109
O	-5.752448	-2.757772	-0.466688
O	-4.104005	-1.182488	-1.451130
O	-3.619871	-2.383396	0.637137
O	-5.360066	-0.618490	0.597701
H	-4.639457	-0.009369	0.976560
H	-2.861549	-1.711446	0.771453
S	4.671078	-1.881384	0.101224
O	5.578247	-2.984782	0.033468
O	5.343943	-0.672041	-0.651483
O	4.194621	-1.438620	1.396307
H	4.658414	0.013918	-0.951566
O	3.421084	-2.225061	-0.799557
H	2.744284	-1.467074	-0.729992
N	-0.172613	3.505676	-0.003871
C	-0.145425	4.278828	-1.266537
C	-0.396161	4.313832	1.216541
H	0.739847	2.967509	0.068016
H	0.603598	5.068622	-1.190730
H	0.135958	3.596433	-2.066957
H	-1.127624	4.717053	-1.450954
H	0.443528	4.995129	1.363729
H	-1.320251	4.884237	1.109242
H	-0.495896	3.627314	2.055202
H	-0.918167	2.753957	-0.052432

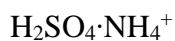


67

S	3.152867	1.927687	0.757211
O	1.761259	2.315381	0.484724
O	3.071687	0.596114	1.687022
O	3.808397	1.459037	-0.497607
O	3.940466	2.862162	1.522147
H	4.239112	-0.111526	-0.541426
N	-0.679840	-1.076988	2.272665
H	0.078274	-1.057336	1.528534
H	-1.579363	-1.301691	1.786121
O	2.837106	-2.883820	0.093957
O	1.556116	-1.829574	-1.698853
S	1.528988	-2.276983	-0.276065
O	1.331532	-1.019430	0.573951
O	0.401134	-3.193131	0.006711
H	-1.143082	-2.784778	-0.578060
H	2.427026	-0.039558	1.260391
H	3.965384	-1.777432	-0.213845
N	4.683405	-1.071640	-0.562440
C	5.844493	-1.034767	0.353259
C	4.993723	-1.422625	-1.966720
C	-0.747664	0.264154	2.902325
C	-0.367040	-2.193320	3.194422
H	-0.276401	-3.100473	2.599267
H	-1.167022	-2.300553	3.928057
H	0.579721	-1.990501	3.695979
H	-1.514901	0.267860	3.678467
H	-0.984086	0.995147	2.131469
H	0.223670	0.504937	3.335241
H	5.620965	-0.647475	-2.409347

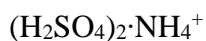
H	5.507517	-2.384538	-1.996992
H	4.047943	-1.503204	-2.500924
H	6.299408	-2.024716	0.411990
H	6.571753	-0.306895	-0.008199
H	5.485053	-0.725432	1.333426
S	-1.574156	3.083457	-0.120618
O	-1.593170	1.572639	-0.177921
O	-0.592503	3.435480	1.098075
O	-1.016661	3.639006	-1.342262
O	-2.869904	3.594089	0.302450
H	-0.241971	0.891178	-1.226044
N	-4.224007	0.792188	-0.207684
H	-3.203077	1.038001	-0.170498
H	-4.278565	-0.229067	-0.471072
O	-1.943883	-2.342028	-0.978104
O	-4.282329	-1.810339	-0.921645
S	-3.286756	-2.530415	-0.100943
O	-3.047111	-1.789506	1.169012
O	-3.528841	-3.941065	0.079206
H	0.323050	3.107457	0.896124
H	0.742736	-0.348274	-1.831913
N	0.202147	0.516290	-2.086172
C	1.130943	1.535584	-2.647832
C	-0.891060	0.117433	-3.008859
C	-4.864170	1.614198	-1.262119
C	-4.796708	0.993178	1.146144
H	-4.336059	0.261898	1.807080
H	-5.873625	0.821443	1.110078
H	-4.576012	2.010513	1.466642
H	-4.714804	2.665977	-1.024862
H	-5.925334	1.367297	-1.316748
H	-4.390848	1.382147	-2.215515
H	-1.478774	1.001185	-3.256200
H	-0.452460	-0.308728	-3.911528
H	-1.506702	-0.632634	-2.513992
H	1.544555	1.148435	-3.580667
H	0.574263	2.455890	-2.814428
H	1.924173	1.713454	-1.925188

Positively charged ammonia-sulfuric acid clusters

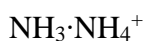


12

H	3.753482	-0.087396	0.945444
S	-0.681440	-0.025187	0.123569
O	-1.375673	-0.943847	-0.969993
O	-1.461063	-0.014165	1.314451
O	-0.675779	1.391217	-0.590636
O	0.711939	-0.393562	0.136213
H	-2.160364	-1.372627	-0.589747
H	-1.542683	1.823734	-0.510432
N	3.366374	-0.032204	0.000108
H	2.315005	-0.097422	0.043749
H	3.731086	-0.807956	-0.558330
H	3.646501	0.852946	-0.428815

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19

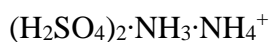
S	1.919215	-0.272124	-0.052576
O	1.856012	1.147228	0.168730
O	1.623659	-1.055378	1.278711
O	1.135895	-0.833155	-1.128114
H	0.832504	2.602849	0.024990
H	0.646815	-1.102509	1.410423
S	-1.919373	-0.271765	0.052571
O	-1.624186	-1.055423	-1.278544
O	-1.136794	-0.833287	1.128411
O	-3.439069	-0.598578	0.231815
O	-1.855041	1.147509	-0.168914
H	-0.647381	-1.103170	-1.410331
H	-3.577255	-1.524024	0.497527
N	0.001063	3.224780	-0.000005
H	-0.830356	2.602884	-0.025335
O	3.438604	-0.600142	-0.232088
H	3.576053	-1.525769	-0.497565
H	-0.021527	3.813895	0.834099
H	0.023609	3.814404	-0.833750

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9

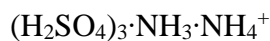
N	1.345451	-0.000039	-0.000025
H	1.733292	0.887206	0.319069
H	1.733813	-0.719610	0.608825
H	1.734374	-0.167164	-0.927515
N	-1.335672	-0.000009	-0.000012
H	-1.695304	0.862191	-0.413384
H	-0.184341	-0.000001	-0.000189
H	-1.695034	-0.073121	0.953416
H	-1.695250	-0.789161	-0.539964

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16

S	0.001296	-0.460925	-0.105845
O	0.000304	-1.455865	1.166249
O	0.003023	0.865666	0.536280
O	-1.229063	-0.729758	-0.856184
O	1.229183	-0.733662	-0.857889
H	0.001320	-2.373630	0.851157
N	-2.800901	1.193797	0.042578
H	-3.534741	0.922798	0.697384
H	-1.993453	1.587236	0.546855
H	-2.382307	0.340514	-0.443148
H	-3.166985	1.864937	-0.632579
N	2.796522	1.196962	0.042791
H	1.979291	1.577990	0.542253
H	2.391515	0.341127	-0.446697
H	3.158352	1.874072	-0.628670
H	3.529346	0.933403	0.701736

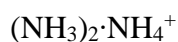


S	-2.120757	-0.163714	0.086989
O	-1.952396	0.870395	-0.902390
O	-1.812977	-1.522725	-0.297389
N	-0.206934	3.054690	-0.925621
H	-0.391477	3.823568	-0.280860
H	-1.011193	2.399093	-0.940985
N	0.647109	-2.795720	-1.041876
H	0.585857	-3.317019	-1.916256
H	-0.275688	-2.393176	-0.797482
S	2.021247	0.106694	0.181573
O	3.326991	-0.047274	1.090753
O	1.807002	1.542230	-0.008413
O	0.997097	-0.559893	1.003847
O	2.251920	-0.620957	-1.071310
H	4.076807	0.394295	0.662223
O	-3.622875	-0.054058	0.545826
H	-3.856119	-0.774126	1.154983
H	-0.043667	3.427815	-1.860905
H	0.633512	2.501608	-0.599110
H	0.945714	-3.419402	-0.291516
H	1.341971	-1.997802	-1.124234
O	-1.382331	0.206974	1.405325
H	-0.394228	-0.062855	1.339634



S	-2.552032	-0.903454	-0.008739
O	-2.576557	0.500927	-0.315567
N	-2.062501	3.225506	-0.965903
H	-2.831476	3.839250	-0.694583
H	-2.300940	2.237804	-0.761042
N	0.348640	-1.239703	2.763788
H	0.581754	-0.240897	2.710492
H	0.977727	-1.740798	2.089077
S	2.000137	-1.486452	-0.458467
O	2.504471	-2.433645	-1.637448
O	0.692272	-1.009258	-1.010950
O	2.939773	-0.386325	-0.312592
O	1.825986	-2.315111	0.729061
H	3.359955	-2.825177	-1.399073
O	-1.797836	-1.716022	-1.103541
H	-0.797491	-1.571389	-1.061258
H	-1.880634	3.322097	-1.966102
H	-1.192292	3.470334	-0.441397
H	0.455611	-1.597876	3.711359
H	-0.621066	-1.346575	2.428732
O	-2.114428	-1.308228	1.305754
S	0.934468	2.129748	0.327612
O	0.385713	1.541511	-1.026961
O	2.474081	2.266933	0.110258
O	0.381937	3.456974	0.398664
O	0.665514	1.199900	1.397393
H	0.543504	0.541773	-1.093541
H	2.856038	1.357194	-0.008938
O	-4.024451	-1.403851	-0.266407

H	-4.126625	-2.334278	-0.006728
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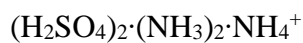
13

N	-2.353209	-0.505375	0.000000
H	-2.380654	-1.195865	0.747972
H	-3.182937	0.073123	0.119282
H	-2.491233	-1.021174	-0.867153
N	-0.000003	1.034017	0.000000
H	0.892603	0.428764	-0.000132
H	-0.892622	0.428784	0.000127
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N	2.353206	-0.505378	0.000001
H	3.182886	0.073144	-0.119514
H	2.380594	-1.196013	-0.747839
H	2.491394	-1.020997	0.867238



20

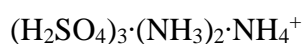
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O	0.214348	1.208862	0.911165
O	1.064800	-0.038573	-1.026342
O	0.115789	-1.244126	0.892421
O	-1.314344	0.052899	-0.612105
N	-1.638400	2.758208	-0.083680
H	-0.808407	2.352016	0.464307
H	-2.373219	3.095869	0.536004
H	-1.949190	1.923186	-0.610125
H	-1.344237	3.499920	-0.717431
N	3.479768	-0.110970	-0.086355
H	2.050751	-0.068840	-0.629950
H	3.658311	0.685083	0.521120
H	4.180583	-0.097249	-0.823131
H	3.632937	-0.951119	0.466123
N	-1.866086	-2.626182	-0.084729
H	-1.634441	-3.388312	-0.720223
H	-2.614823	-2.909555	0.545398
H	-0.999323	-2.279146	0.451938
H	-2.124822	-1.774502	-0.610209



27

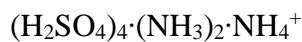
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O	1.560829	0.440145	-1.233462
N	-0.013134	-2.328094	-1.377575
H	0.904099	-2.147965	-0.902575
H	-0.739716	-2.280953	-0.640379
O	2.034699	-1.467053	0.217829
O	1.834018	0.773252	1.180012
N	-0.077755	2.569861	-1.101384
H	0.356263	3.438630	-0.793310
H	0.647667	1.805408	-1.195630
N	-0.191669	-0.112973	2.761997

H	0.054540	-0.646247	3.594228
H	0.669375	0.209545	2.245139
S	-2.139270	-0.006976	-0.069571
O	-3.718970	-0.245559	0.092732
O	-1.816381	0.032394	-1.488872
O	-1.586608	-1.189162	0.628982
O	-1.806084	1.245070	0.634254
H	-4.203153	0.423009	-0.415389
O	3.755372	0.250685	-0.287010
H	4.288014	-0.083816	0.450703
H	-0.781065	2.232903	-0.404596
H	-0.539605	2.709449	-1.999252
H	-0.212639	-1.546341	-2.009216
H	-0.023868	-3.216116	-1.875699
H	-0.755940	-0.683655	2.091961
H	-0.752446	0.701664	3.012582



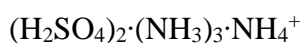
34

S	-2.680907	-1.374538	-0.001954
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O	-3.874549	-2.441317	-0.121617
O	-3.021668	-0.399657	-1.043434
H	-3.721289	-3.169645	0.499328
S	2.971559	-1.134350	0.067211
O	3.565798	0.302541	0.055299
O	4.198795	-1.963414	0.614959
O	1.932857	-1.242224	1.055855
H	4.795193	-2.205344	-0.111713
S	0.422016	2.284797	-0.132646
O	-0.711940	2.042420	0.783499
O	0.273899	1.642976	-1.433468
O	1.707903	2.027744	0.521518
H	-2.386223	2.200208	0.339047
O	-1.422294	-2.081452	-0.260811
N	0.064557	-1.039191	-2.316378
N	-3.373048	2.021186	0.043480
N	-0.302252	-0.185532	2.481244
H	-3.972287	1.952263	0.865227
H	-3.707917	2.765077	-0.566902
H	-3.364310	1.086449	-0.456935
H	2.847243	1.001488	0.201707
H	-1.210150	-0.600625	2.164452
H	-0.228335	-0.187442	3.496979
H	0.489600	-0.698636	2.064922
H	-0.288957	0.780069	2.107944
H	-0.553183	-1.521947	-1.619845
H	1.030667	-1.374237	-2.187858
H	0.052799	-0.024009	-2.106810
H	-0.262039	-1.212908	-3.265083
O	2.686117	-1.568542	-1.280511
O	0.311369	3.870557	-0.361722
H	1.063398	4.175863	-0.892377



41

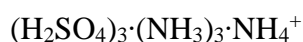
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O	1.364756	2.108774	1.403007
O	2.592611	3.441038	-0.293539
O	2.066149	1.168708	-0.754295
H	2.342489	4.267378	0.146874
S	-4.786312	-0.153956	-0.492780
O	-4.514489	1.251703	-0.381657
O	-3.942397	-0.792136	-1.654132
O	-4.676530	-0.985103	0.683914
H	-3.002061	-0.910220	-1.321746
S	-1.244961	-1.240035	0.828906
O	0.069758	-1.847190	0.976854
O	-1.526566	-0.924907	-0.609951
O	-1.469647	-0.077188	1.688138
O	-2.272167	-2.369758	1.255029
H	-3.182253	-2.000653	1.236105
O	0.225462	2.782180	-0.652318
N	1.862230	-0.418837	2.545233
N	-2.154115	2.417298	0.763663
N	0.844719	-0.943186	-2.074334
H	-1.909251	1.510738	1.222182
H	-3.005254	2.254650	0.207834
H	-2.329789	3.134319	1.465250
H	-1.344937	2.686172	0.167117
H	0.725704	-1.001308	-3.084288
H	-0.061631	-1.101352	-1.582612
H	1.560338	-1.613758	-1.764540
H	1.194221	-0.005051	-1.795250
H	1.140313	-1.030808	2.106551
H	1.691854	0.557856	2.228913
H	2.784835	-0.722788	2.199455
H	1.817848	-0.480117	3.560753
S	4.376352	-1.150043	-0.379848
O	4.568521	0.337469	-0.840869
O	5.842664	-1.686937	-0.586504
O	4.135965	-1.222037	1.033931
O	3.468287	-1.822995	-1.279296
H	6.027381	-1.827887	-1.529085
H	3.679163	0.799547	-0.829785
O	-6.232758	-0.263098	-1.105806
H	-6.573754	-1.167494	-1.011727



31

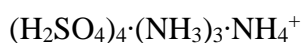
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H	0.719948	-1.934475	-1.044417
H	-0.934417	-2.139156	-0.824954
O	1.875925	-1.226271	-0.014546
O	1.416453	0.927798	1.062323
N	-0.705876	2.638222	-0.812602
H	-0.246502	3.421647	-0.350541
H	0.014326	1.893172	-1.070573
N	-0.437610	-0.196130	2.637884
H	-0.117367	-0.660533	3.485036
H	0.372012	0.215043	2.083439
S	-2.587535	-0.172053	0.006219

O	-4.121025	-0.580102	0.266759
O	-2.391206	0.022095	-1.419930
O	-1.871754	-1.346383	0.553844
O	-2.317556	1.042792	0.802744
H	-4.702486	0.066952	-0.160141
O	3.253482	0.740310	-0.555533
H	4.036538	0.184643	-0.106073
H	-1.389413	2.180866	-0.168605
H	-1.189186	2.962011	-1.648577
H	-0.379556	-1.282732	-2.119889
H	-0.169756	-2.954565	-2.113971
H	-0.947804	-0.848778	2.005224
H	-1.094964	0.552636	2.859385
N	5.210706	-0.614074	0.457412
H	4.934160	-1.589554	0.537670
H	5.499349	-0.299336	1.380076
H	6.028007	-0.573320	-0.146932

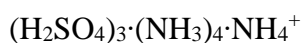


38

S	2.206788	-1.858397	-0.044660
O	1.056851	-1.251929	-0.756932
O	2.247222	-3.311476	-0.760452
O	3.478354	-1.207395	-0.332600
H	2.964508	-3.835353	-0.372500
S	-3.144821	-0.490856	0.206796
O	-3.192381	0.821634	0.852719
O	-4.637569	-1.099046	0.244278
O	-2.863170	-0.437403	-1.232900
H	-4.967364	-1.076044	1.155238
S	0.947881	2.351266	-0.039446
O	1.225256	1.586273	1.187932
O	2.192194	2.738871	-0.712227
O	-0.022578	3.427772	0.095132
O	0.169221	1.323972	-1.029929
H	0.612998	0.445700	-1.010401
O	1.948541	-2.086762	1.371738
N	-0.104211	-0.488538	2.407834
N	-2.431110	2.754167	-0.951481
N	-1.186242	-2.558324	-1.623935
N	4.322232	1.384382	0.121473
H	-1.499192	-3.195619	-0.891115
H	-1.871648	-1.760141	-1.651114
H	-0.252736	-2.168982	-1.348781
H	-1.131707	-3.043955	-2.517417
H	-3.070453	3.494037	-1.234502
H	-1.533331	3.144170	-0.564183
H	-2.859020	2.134124	-0.227378
H	-2.196309	2.157799	-1.746202
H	4.059210	0.382163	-0.006471
H	4.486641	1.570652	1.109600
H	5.165068	1.595818	-0.410545
H	3.506061	1.983848	-0.217381
H	0.628079	-1.193714	2.196475
H	-0.985019	-0.775891	1.933408
H	0.241983	0.415114	2.013619
H	-0.250953	-0.406693	3.411583
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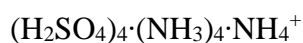
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45

S	1.593979	2.217709	0.903242
O	2.185478	3.002106	-0.187406
O	0.519341	1.205671	0.233919
O	2.609480	1.364407	1.546369
O	0.752657	2.980415	1.813281
H	0.985617	0.533318	-0.314291
S	3.040922	-1.428443	-1.128166
O	1.654354	-0.919677	-1.028090
O	2.833953	-2.600115	-2.229395
O	3.973238	-0.466175	-1.703342
O	3.511013	-2.066897	0.094900
H	3.676664	-3.059600	-2.363442
S	-3.371190	0.813976	-1.670414
O	-3.122722	2.047688	-0.962831
O	-2.281986	0.150371	-2.331705
O	-4.137262	-0.184071	-0.748190
N	-1.911116	2.396762	1.652111
H	-2.488760	2.999552	2.235218
H	-1.995726	1.412282	1.967881
H	-0.904717	2.690212	1.709147
H	-2.239679	2.436878	0.676795
N	2.171111	-1.201770	2.394303
H	2.302606	-0.174959	2.236578
H	2.698935	-1.685740	1.641212
H	1.167050	-1.437423	2.296144
H	2.516099	-1.477177	3.311170
N	-0.693978	-2.147093	-1.772833
H	-1.178676	-1.434840	-2.334194
H	-1.259514	-2.259830	-0.908112
H	-0.618233	-3.024984	-2.283015
H	0.255476	-1.788595	-1.521166
N	4.586460	2.105383	-0.905926
H	5.022642	2.640898	-1.654824
H	4.415826	1.122862	-1.217191
H	5.194775	2.100578	-0.088396
H	3.647530	2.533577	-0.634125
S	-1.859006	-1.583666	1.729800
O	-2.270453	-0.317835	2.322412
O	-2.464034	-2.749266	2.653917
O	-0.440531	-1.882834	1.707065
H	-3.381721	-2.537566	2.881797
O	-4.467541	1.088502	-2.778205
O	-2.457903	-1.776949	0.372860
H	-5.035815	1.827576	-2.510679
H	-3.499674	-0.805945	-0.255974

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42

S	-1.416896	1.951286	-0.110997
O	-1.817642	1.650493	1.295280
O	-2.725835	1.615672	-0.988633
O	-1.109681	3.349090	-0.340828

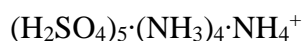
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O	-0.907636	-2.221979	0.206645
O	-2.882415	-3.352538	-0.758905
O	-3.136862	-1.607009	0.983736
O	-2.451826	-1.066614	-1.318642
H	-2.814760	-4.034942	-0.074155
N	1.765383	3.107963	-0.594378
H	2.350059	3.937065	-0.677410
H	2.012687	2.547768	0.254556
H	1.966701	2.436956	-1.349781
H	0.757665	3.352778	-0.582433
N	0.571980	-1.100331	-2.038105
H	-0.183047	-0.423540	-1.861232
H	0.488709	-1.801678	-1.291123
H	1.477510	-0.582182	-1.930951
H	0.471133	-1.534943	-2.952256
N	0.184859	-0.273577	2.053341
H	1.079980	0.155476	1.717025
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H	0.289272	-0.606379	3.009425
H	-0.562719	0.440057	1.986715
N	-4.380293	0.765014	1.360280
H	-4.966560	0.821379	2.190929
H	-4.090197	-0.227685	1.167549
H	-4.870107	1.152967	0.554329
H	-3.476599	1.289366	1.479326
S	3.029801	0.061252	0.019800
O	4.571028	0.156261	0.160367
O	2.686302	0.528639	-1.351140
O	2.451663	1.006023	1.028297
O	2.595694	-1.313212	0.263109
N	5.632525	-2.117662	0.733589
H	4.850757	-2.764858	0.794330
H	6.272424	-2.460223	0.023055
H	5.021698	-0.778391	0.397527
H	6.123056	-2.129164	1.623234



49

S	-1.460159	2.029528	0.182555
O	-1.424976	1.164689	1.401868
O	-3.007845	2.243222	-0.117809
O	-0.924314	3.360416	0.425839
O	-0.860588	1.357982	-0.977579
H	-3.375896	1.436104	-0.597309
S	-4.367121	-1.093633	-0.422808
O	-3.343211	-2.111828	-0.242360
O	-5.478480	-1.841243	-1.308004
O	-5.044706	-0.668079	0.811914
O	-3.896285	0.055489	-1.223104
H	-6.240206	-1.254198	-1.424065
S	1.978908	-2.647644	0.227778
O	3.388265	-2.953628	0.003911
O	1.465390	-1.546702	-0.613399
O	1.128312	-3.889093	-0.365524
N	1.132503	3.641270	-1.405698

H	1.155230	4.414979	-2.066490
H	2.062211	3.512241	-0.934284
H	0.928999	2.757909	-1.881442
H	0.378700	3.766936	-0.696865
N	-1.123821	-1.350485	-1.695157
H	-1.159206	-0.323490	-1.546105
H	-1.908971	-1.777757	-1.151993
H	-0.201641	-1.674998	-1.355911
H	-1.239330	-1.567102	-2.682954
N	1.033240	0.101969	2.359417
H	1.862814	0.529300	1.882967
H	1.099927	-0.922730	2.181448
H	1.084061	0.285825	3.359254
H	0.146281	0.485688	1.976322
N	-4.000896	1.144469	2.454965
H	-4.163982	0.923857	3.435588
H	-4.455423	0.413388	1.826092
H	-4.387101	2.061721	2.232862
H	-2.979897	1.161425	2.228788
S	3.591207	1.423101	-0.230209
O	4.824937	0.926268	-0.846829
O	2.359759	0.969940	-1.185290
O	3.459768	2.873046	-0.230501
H	2.137858	0.022091	-1.026826
O	1.612827	-2.513807	1.636086
O	3.346297	0.766520	1.067117
H	1.291340	-4.675339	0.176865
N	5.637048	-1.390802	0.188289
H	4.795599	-2.012174	0.149081
H	6.406495	-1.812306	-0.329595
H	5.375384	-0.447928	-0.235269
H	5.913673	-1.255548	1.159385

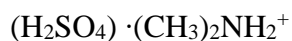


56

S	3.311783	-0.540943	0.946250
O	3.887567	-0.216507	-0.360126
O	3.511697	-2.099700	1.212440
O	3.992334	0.101820	2.064012
O	1.834873	-0.322337	0.960671
H	3.092496	-2.609606	0.478794
S	0.824818	-3.405575	-1.453934
O	1.823619	-3.506508	-0.375501
O	0.785306	-4.843210	-2.181213
O	-0.529243	-3.298493	-0.903691
O	1.152258	-2.422069	-2.479192
H	1.652102	-5.022273	-2.575310
S	-3.025477	-1.148669	1.883142
O	-2.103161	-0.007475	1.973678
O	-2.359656	-2.425390	2.103422
O	-4.136643	-0.969073	3.029005
N	4.786154	2.591531	1.284971
H	5.680763	2.577104	0.797656
H	4.013405	2.841390	0.602308
H	4.821051	3.270854	2.043160
H	4.577157	1.631930	1.664428
N	0.442157	-2.549331	1.974876
H	0.832148	-1.614657	1.734195

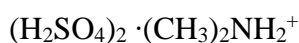
H	0.755189	-3.187729	1.227654
H	-0.597420	-2.519163	2.012532
H	0.822856	-2.853298	2.869236
N	-2.885275	-2.284143	-1.693921
H	-2.710918	-1.328400	-2.034935
H	-3.394715	-2.171752	-0.800126
H	-3.426833	-2.826403	-2.363603
H	-1.957759	-2.742134	-1.495887
N	2.087818	0.234805	-2.409941
H	2.482674	0.499358	-3.309609
H	1.448019	0.987164	-2.067157
H	1.604392	-0.677074	-2.489102
H	2.848328	0.119682	-1.704922
S	1.376877	3.039982	-0.265301
O	0.864063	4.393923	-0.038307
O	1.121273	2.317322	1.141723
O	2.829294	2.998204	-0.501898
H	1.313744	1.348847	1.064915
O	-3.858426	-1.112524	0.663555
O	0.630858	2.301770	-1.290347
H	-3.720921	-1.066716	3.898772
N	-1.611329	5.033009	-0.714652
H	-2.106377	5.308345	0.132706
H	-0.610787	4.745121	-0.458574
H	-2.113174	4.232778	-1.148060
H	-1.592064	5.818973	-1.362852
S	-2.929470	1.617941	-0.999882
O	-2.230794	2.019552	0.343903
O	-4.385625	1.196361	-0.576932
O	-2.264739	0.486463	-1.601681
O	-3.055454	2.842500	-1.743010
H	-2.119801	1.238325	0.975474
H	-4.341928	0.337434	-0.069496

Positively charged ammonia-sulfuric acid clusters

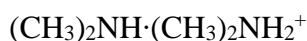


18

H	-2.696159	0.014717	-1.437322
S	1.347121	0.028635	0.003181
O	2.472549	-0.041593	-1.109667
O	1.108724	1.408694	0.254558
O	2.016112	-0.678890	1.257546
O	0.264400	-0.855871	-0.363164
H	2.594261	-0.952942	-1.425941
H	2.649337	-0.078067	1.686884
N	-2.426603	-0.043369	-0.453004
H	-1.438121	-0.364919	-0.442704
C	-3.281284	-1.068493	0.232870
H	-4.320280	-0.745248	0.201826
H	-2.946601	-1.159330	1.264408
H	-3.165476	-2.021614	-0.280124
C	-2.491092	1.328013	0.156054
H	-3.512181	1.699058	0.089244
H	-1.807985	1.982947	-0.381402
H	-2.184546	1.254976	1.197548

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25

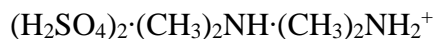
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O	-1.725237	-1.453297	-1.284482
O	-1.247180	-1.303404	1.128834
H	0.971555	2.075355	-0.033211
H	-0.752033	-1.568636	-1.405444
S	1.856489	-0.945064	-0.058156
O	1.481932	-1.681552	1.281136
O	1.033131	-1.454203	-1.131326
O	3.341080	-1.419381	-0.223964
O	1.922213	0.475301	0.140593
H	0.500990	-1.657041	1.394959
H	3.388136	-2.358928	-0.470121
N	0.210604	2.770173	-0.005952
H	-0.645901	2.196986	0.000976
C	0.240670	3.602878	-1.249279
H	1.179741	4.152417	-1.284312
H	-0.598528	4.295968	-1.230555
H	0.159965	2.944631	-2.112457
C	0.302779	3.551010	1.267804
H	1.236858	4.109983	1.272650
H	0.281370	2.855836	2.105105
H	-0.543070	4.233769	1.326281
O	-3.519463	-0.902380	0.220601
H	-3.714446	-1.820807	0.473717

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21

N	-1.312253	0.000101	-0.370481
H	-1.354994	0.000601	-1.387769
C	-1.987356	-1.228254	0.108635
C	-1.987816	1.227703	0.109848
H	-1.901278	-1.289642	1.195695
H	-3.050935	-1.238795	-0.149874
H	-1.513198	-2.106917	-0.331621
H	-1.901875	1.287937	1.196981
H	-3.051369	1.238159	-0.148780
H	-1.513885	2.106994	-0.329399
N	1.321622	0.000139	0.373097
H	1.334772	0.000621	1.394015
H	0.248301	-0.000217	0.067510
C	1.976299	-1.250728	-0.116472
C	1.975360	1.251048	-0.117602
H	3.022073	1.266176	0.184361
H	1.457658	2.112242	0.302279
H	1.908486	1.276178	-1.204502
H	3.023004	-1.264823	0.185573
H	1.459212	-2.111942	0.304118
H	1.909526	-1.276857	-1.203355

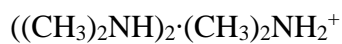


S	0.093795	-0.181845	-0.001433
O	-0.902850	0.888078	-0.001331
O	0.900018	-0.275985	-1.217770
O	0.900099	-0.275581	1.215024
N	3.354843	0.174368	-0.000146
H	2.706317	0.020580	-0.795594
H	2.702441	0.021126	0.792521
C	4.436799	-0.851108	0.002902
C	3.832061	1.588251	0.000420
H	5.051483	-0.725747	-0.887220
H	5.046889	-0.725049	0.896074
H	3.981451	-1.839871	0.002139
H	4.433823	1.762142	-0.890327
H	4.429601	1.762755	0.893879
H	2.965886	2.247498	-0.001843
N	-3.428898	0.008308	0.000773
H	-3.186754	-0.985657	-0.000102
H	-2.481561	0.474110	0.000026
C	-4.154696	0.351238	1.259267
C	-4.157473	0.352876	-1.255660
H	-5.106142	-0.181326	-1.286089
H	-3.538394	0.070449	-2.105390
H	-4.334172	1.427019	-1.272071
H	-5.103271	-0.183048	1.291096
H	-3.533719	0.067723	2.107248
H	-4.331393	1.425351	1.277454
O	-0.904835	-1.504943	-0.001159
H	-0.364410	-2.307345	-0.002957



S	0.638213	2.087620	-0.224616
C	-3.951129	0.400821	-0.497005
H	-4.736007	-0.321515	-0.278288
H	-4.385016	1.386511	-0.658489
H	-3.386022	0.084772	-1.371255
O	-0.770027	2.246891	0.057359
O	1.522234	1.734904	0.854946
N	-3.011997	0.460799	0.663300
C	-3.639993	0.874025	1.951867
H	-2.560412	-0.473840	0.772028
H	-2.240488	1.104570	0.434766
H	-4.071127	1.867693	1.839611
H	-2.874939	0.887434	2.726269
H	-4.417346	0.157913	2.213557
C	3.931299	-0.691137	-0.529606
H	3.392243	-0.275693	-1.379064
H	4.239323	-1.712328	-0.747661
H	4.802019	-0.077440	-0.303415
N	3.015773	-0.702279	0.650120
C	3.622946	-1.234862	1.905206
H	2.168621	-1.261899	0.416113
H	2.657229	0.251670	0.811320
H	2.874343	-1.203903	2.694857
H	3.937667	-2.263398	1.736676
H	4.480247	-0.621811	2.179314

S	-0.647213	-1.915341	-0.341326
O	-1.030536	-3.094670	-1.360456
O	-0.832842	-0.719388	-1.194514
O	0.738099	-2.130735	0.069391
O	-1.610187	-1.946111	0.757320
H	-1.022531	-3.940053	-0.885599
O	0.837384	1.119233	-1.427435
H	0.162183	0.326211	-1.381826
O	1.229713	3.431666	-0.811599
H	0.648134	3.791612	-1.500647



31

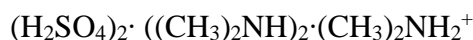
N	-2.279242	-0.665080	-0.355486
H	-2.213356	-1.042365	-1.298274
C	-2.287234	-1.804189	0.584222
C	-3.524957	0.124789	-0.274813
H	-2.307992	-1.429332	1.610128
H	-3.157449	-2.456398	0.445354
H	-1.382106	-2.399871	0.451617
H	-3.593973	0.596288	0.708233
H	-4.421199	-0.490248	-0.417978
H	-3.517602	0.907617	-1.035466
N	0.003927	1.010862	0.011785
H	0.895370	0.449453	-0.173012
H	-0.830983	0.356092	-0.125209
C	-0.082424	2.108628	-0.989469
C	0.016668	1.493509	1.419889
H	0.876143	2.144784	1.577310
H	0.082262	0.637037	2.089724
H	-0.898946	2.047340	1.626264
H	0.781081	2.766255	-0.890275
H	-0.097468	1.677807	-1.990150
H	-0.994309	2.682683	-0.827285
N	2.422474	-0.427678	-0.482373
C	2.220005	-1.883632	-0.348995
C	3.523264	0.057863	0.374612
H	2.676227	-0.237294	-1.449209
H	1.884501	-2.112466	0.665352
H	1.453391	-2.216207	-1.051681
H	3.136373	-2.454790	-0.538863
H	3.254763	-0.079366	1.424567
H	4.462797	-0.477157	0.192936
H	3.690430	1.121604	0.195759



38

S	0.000007	-0.143982	0.000031
O	0.537025	-0.999098	-1.096385
O	-1.111321	0.732080	-0.526924
O	-0.537029	-0.998979	1.096531
N	-2.910271	-1.353893	-0.078223
H	-2.698968	-0.421043	-0.472430
H	-2.090588	-1.435763	0.585075
C	-4.210168	-1.367198	0.639101
C	-2.761858	-2.377335	-1.152106

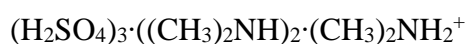
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H	-4.348054	-2.338993	1.111548
H	-4.199204	-0.589712	1.401455
H	-3.532229	-2.226451	-1.907744
H	-2.862425	-3.369002	-0.712711
H	-1.771300	-2.259884	-1.589694
N	2.910444	-1.353581	0.078148
H	2.699021	-0.420697	0.472226
H	2.090747	-1.435662	-0.585094
C	2.762206	-2.376870	1.152201
C	4.210316	-1.366829	-0.639221
H	5.020907	-1.183665	0.065675
H	4.199218	-0.589475	-1.401709
H	4.348322	-2.338686	-1.111508
H	3.532586	-2.225759	1.907785
H	1.771651	-2.259480	1.589813
H	2.862887	-3.368595	0.712963
O	1.111325	0.732143	0.526889
H	0.707642	2.417444	0.338028
N	-0.000152	3.112746	-0.000009
C	0.535568	3.908100	-1.133732
C	-0.536095	3.907992	1.133684
H	-0.707764	2.417218	-0.338017
H	1.358528	4.531748	-0.785414
H	0.889737	3.221716	-1.901098
H	-0.254224	4.538210	-1.541870
H	0.253493	4.538405	1.541748
H	-1.359287	4.531328	0.785356
H	-0.889999	3.221536	1.901109



45

S	1.884192	-0.076190	-1.260217
O	0.951264	-1.204906	-1.232511
C	1.042951	3.292035	0.938365
H	1.802628	4.005117	0.620381
H	0.433800	3.723448	1.731465
H	1.519539	2.376014	1.279270
N	1.521374	-1.389638	2.123490
H	1.998933	-0.861259	1.361622
H	0.581763	-0.940556	2.185830
C	2.241720	-1.188110	3.410381
C	1.373519	-2.814923	1.714848
H	2.359753	-3.273897	1.655605
H	0.898954	-2.835042	0.736946
H	0.761697	-3.337330	2.449023
H	3.254439	-1.579415	3.322844
H	2.275151	-0.122545	3.630836
H	1.709881	-1.708627	4.205766
O	2.456970	0.217815	0.063064
O	1.375776	1.124501	-1.930099
N	0.171397	2.954684	-0.222056
C	-0.471985	4.127970	-0.874171
H	0.721272	2.408753	-0.918350
H	-0.569185	2.282482	0.077953
H	-1.104045	4.639576	-0.149497
H	-1.079966	3.777218	-1.706259
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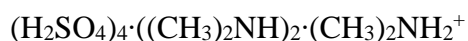
C	-1.796846	-2.907914	-2.471055
H	-1.248354	-3.583397	-1.817122
H	-1.365662	-2.937018	-3.470797
H	-2.845416	-3.200224	-2.509169
N	-1.689306	-1.524892	-1.930431
C	-2.392506	-0.488984	-2.737891
H	-0.681841	-1.280328	-1.831735
H	-2.037808	-1.495436	-0.949050
H	-2.302412	0.460041	-2.214893
H	-1.934298	-0.430175	-3.724327
H	-3.443249	-0.761168	-2.830956
S	-1.882255	0.065593	1.271585
O	-3.204123	0.595095	2.031956
O	-1.744914	1.038112	0.182005
O	-2.167756	-1.293028	0.799337
O	-0.788564	0.116101	2.249718
H	-3.411555	-0.010532	2.758960
O	3.079510	-0.646624	-2.182800
H	3.706275	0.069947	-2.361405



52

S	-3.223059	-1.004714	0.110782
O	-3.184802	0.459256	0.205771
O	-4.801166	-1.303294	0.076695
O	-2.678452	-1.515797	-1.160938
H	-4.941985	-2.256714	-0.026235
S	1.733615	1.848743	0.237608
O	2.541427	1.147581	1.237488
O	1.922958	1.370081	-1.135131
S	0.670184	-1.798101	-1.018165
O	0.513655	-0.639843	-2.092256
O	0.443194	-1.232439	0.293713
O	1.937317	-2.467920	-1.212688
O	-0.456124	-2.747908	-1.452884
H	-1.374460	-2.316114	-1.301735
O	-2.664235	-1.669330	1.286508
H	1.054684	0.144457	-1.789548
O	0.312153	1.959279	0.617489
O	2.304465	3.355495	0.142584
H	2.431112	3.700276	1.039002
N	-0.886784	0.055050	2.546485
H	-0.392029	0.591122	1.816261
H	-1.456961	-0.661745	2.046037
C	0.110598	-0.629321	3.415628
C	-1.818305	0.963734	3.273213
H	-0.418240	-1.206730	4.172718
H	0.703921	-1.288156	2.787450
H	0.747598	0.116849	3.888219
H	-2.345780	0.391803	4.035072
H	-1.250054	1.769637	3.735577
H	-2.534089	1.357628	2.555024
N	4.004477	-1.020943	0.108496
H	3.290155	-1.618601	-0.349857
H	3.478811	-0.256067	0.578110
C	4.738637	-1.826186	1.126743

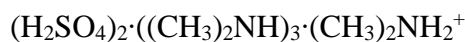
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H	5.448816	-1.184570	1.646021
H	4.020165	-2.235195	1.835013
H	5.265173	-2.638573	0.628221
H	5.621349	0.214471	-0.470459
H	5.359321	-1.216456	-1.506918
H	4.247106	0.180727	-1.603634
N	-1.815110	2.198579	-1.349243
H	-0.913778	2.123521	-0.849334
H	-2.427250	1.498950	-0.865812
C	-2.366421	3.565607	-1.129927
C	-1.664185	1.819454	-2.785110
H	-3.361711	3.621524	-1.567859
H	-2.424850	3.751588	-0.059163
H	-1.710864	4.299073	-1.597573
H	-2.634771	1.903954	-3.271791
H	-0.948482	2.488817	-3.260808
H	-1.313492	0.791232	-2.838144



59

S	-2.372696	-1.285476	0.060031
O	-2.185594	-2.771377	-0.427973
O	-3.635252	-1.284841	0.781648
O	-1.190933	-0.972703	0.916234
O	-2.398900	-0.402898	-1.123994
H	1.492321	3.756597	-0.035383
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H	-0.085555	-2.232021	1.663919
H	1.414193	-2.787449	1.324723
O	2.247073	0.859336	-0.717669
O	2.016490	-0.251362	1.484939
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O	3.652354	1.581058	1.069953
O	4.042494	-0.629489	0.148068
H	3.583333	-1.490429	-0.061316
H	-4.585655	0.113205	0.311719
H	2.958306	3.123306	0.414504
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C	3.006404	4.126869	-1.399000
C	0.098891	-4.303130	1.843574
C	1.054339	-2.562077	3.372484
H	1.431414	-1.543116	3.368327
H	1.836243	-3.251765	3.687524
H	0.194494	-2.650942	4.034944
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H	0.860127	-5.004424	2.182177
H	-0.130198	-4.479212	0.795979
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H	4.079161	4.312071	-1.373801
H	2.798833	3.208925	-1.944485
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H	2.343148	4.909425	1.874773
S	-1.079870	2.430002	-0.063517
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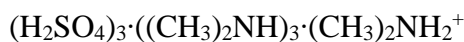
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C	-5.514579	0.873137	-1.386178
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H	-6.747111	0.928402	1.085450
H	-5.375840	1.672442	1.947602
H	-6.220502	2.581502	0.668113
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H	-5.823999	1.846445	-1.764557
H	-4.742356	0.444325	-2.021292
S	1.469992	-2.570532	-1.523705
O	2.366907	-2.667208	-0.356305
O	0.233173	-3.332942	-1.358936
H	-1.317764	-2.887298	-0.902975
O	1.243539	-1.189585	-1.963017
H	1.811543	0.087194	-1.203172
O	2.326650	-3.305445	-2.663233
H	1.803267	-3.349708	-3.478058



55

S	-1.420686	-0.013292	0.876741
O	-2.709473	-0.019954	1.622558
O	-0.613277	-1.226876	1.198038
O	-0.631687	1.205635	1.219415
O	-1.722794	-0.027408	-0.613129
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H	0.900100	-1.794940	-1.203061
H	-0.653456	-1.205734	-1.314184
O	3.056335	0.705923	0.449505
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O	2.525993	-1.457107	-0.553097
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C	-0.544769	-3.279735	-1.256581
C	1.298528	0.199942	3.722023
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H	-0.693343	-3.250422	-0.179553
H	-1.493828	-3.459642	-1.761676
H	-1.129263	2.404990	-1.901256
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H	-0.032273	3.716062	-2.431186
H	2.195309	3.175486	0.519534
H	1.924132	4.277311	-0.851707
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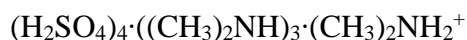
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H	-0.779519	-1.884304	-3.645132
H	0.854527	-2.581397	-3.498353
C	2.426408	-1.859975	2.849816
H	1.824229	-2.510100	3.483564
H	3.347089	-1.590577	3.367342
H	2.660882	-2.358630	1.911321
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H	-3.915982	0.011022	0.692317
C	-5.330470	-1.213802	-0.307014
C	-5.317748	1.287855	-0.262270
H	-5.845948	1.353721	-1.213779
H	-6.035267	1.297128	0.557343
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H	-6.048715	-1.244990	0.511403
H	-5.858821	-1.240688	-1.260373
H	-4.658669	-2.066864	-0.227375
O	4.306037	-0.039489	-1.557888
H	4.981307	-0.399902	-0.964846



62

S	3.032820	0.661807	-0.113686
O	3.350035	-0.599533	0.580378
O	4.356585	1.597309	-0.016618
O	2.778380	0.450623	-1.541293
H	5.070967	1.179799	-0.519015
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O	-2.090310	-2.547296	-0.120862
O	-0.410280	-1.069218	-1.184814
O	-0.739211	-1.064805	1.266173
H	-1.080503	-0.321581	-1.262381
S	-2.445001	1.775477	-0.151720
O	-2.203531	3.135340	-0.612472
O	-2.243233	0.738261	-1.192134
O	-3.705260	1.554721	0.555155
O	-1.238667	1.568602	0.909117
H	-1.112691	0.606595	1.097712
O	2.039604	1.468566	0.588843
O	0.347191	-2.928286	0.107782
N	0.518059	3.644141	-0.374281
H	0.934756	2.752785	-0.046644
H	-0.492492	3.458415	-0.559682
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C	1.202637	4.055822	-1.630191
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H	0.057399	4.239042	1.585585
H	1.651158	4.789001	0.996320
H	0.736379	4.961904	-2.014715
H	2.256450	4.234520	-1.420809
H	1.108305	3.250583	-2.356680
N	1.642328	-1.185807	2.685752
H	2.337459	-1.006967	1.929555
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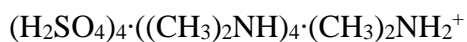
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H	0.958536	-0.208864	4.434737
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H	1.620982	0.857843	3.160161
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H	-6.299210	-1.054796	1.108664
H	-5.287338	-2.036346	-1.694160
H	-6.000609	-0.435824	-1.345754
H	-4.356344	-0.543994	-2.024526



69

S	-2.141725	-2.245959	-0.340778
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O	-2.421891	-1.085948	-1.228578
O	-1.448698	-3.358688	-1.236861
H	-4.664152	-1.764375	-0.042790
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S	-2.562379	1.881271	0.383805
O	-1.803345	1.310776	-0.850066
O	-2.373041	3.314240	0.335027
O	-1.835470	1.266983	1.619522
H	-1.988940	0.298616	-0.983606
N	-5.350996	-0.981846	-0.168754
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H	-7.126621	-0.260424	0.729913
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C	-5.798709	-0.970895	-1.589956
H	-6.325205	-1.900060	-1.803627
H	-4.913247	-0.893946	-2.217610
H	-6.458607	-0.119893	-1.754712
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O	3.116703	-2.000777	-0.000554
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H	0.263139	-2.018117	3.839395
H	2.045057	-2.088755	3.814263
H	1.186406	-0.738559	3.006682



79

S	-2.966122	2.112272	-0.359731
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O	-4.247648	2.184809	0.353956
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O	-1.656411	-3.135359	0.440385
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N	-0.238765	4.574631	0.130447

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H	0.467800	5.286595	-1.719664
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O	1.970879	-3.116605	-0.211321
H	5.122429	-0.489301	-0.240592
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O	3.013956	1.220164	1.239394
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N	0.235961	-2.934725	2.472403
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H	-1.395715	-4.385618	-3.128924
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H	-5.359680	0.196109	-2.094655
H	-6.737901	-0.883634	-1.722881
H	-6.908355	0.886152	-1.551244

References

- Becke, A.D., *J. Chem. Phys.* **98**, 5648 (1993).
Frisch, M.J., et al. Gaussian 09, Revision A.01, (2009).
Lide, D., ed.: CRC Handbook of Chemistry and Physics, 91th Edition, CRC Press/Taylor and Francis, Boca
Montgomery Jr, J. A., et al., *J. Chem. Phys.* **110**, 2822 (1999).
Nadykto, A.B., and Yu, F., *J. Geophys. Res.* **108**, 4717 (2003).
Sedo, G., et al. *J. Mol. Spectrosc.* **251**, 4 (2008).