

Supplementary material for:

Amine substitution into sulfuric acid - ammonia clusters

Oona Kupiainen, Ismael K. Ortega, Theo Kurtén and Hanna Vehkamäki

Division of Atmospheric Sciences, Department of Physics, P.O. Box 64, FI-00014 University of Helsinki, Finland.

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

$[\text{H}_2\text{SO}_4 \cdot \text{NH}_4]^+$

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

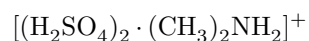
$[\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH}_2]^+$

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

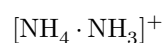
$[(\text{H}_2\text{SO}_4)_2 \cdot \text{NH}_4]^+$

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



S	-1.978644	-0.668544	0.056018
O	-1.817112	0.744372	-0.140500
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

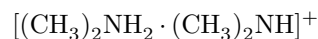


N	1.345451	-0.000039	-0.000025
H	1.733292	0.887206	0.319069
H	1.733813	-0.719610	0.608825
H	1.734374	-0.167164	-0.927515
N	-1.335672	-0.000009	-0.000012
H	-1.695304	0.862191	-0.413384
H	-0.184341	-0.000001	-0.000189
H	-1.695034	-0.073121	0.953416
H	-1.695250	-0.789161	-0.539964

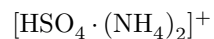


H	0.626694	0.000070	-1.416776
H	-2.718852	0.865278	-0.244890
N	0.496381	0.000194	-0.403398
H	-0.569503	0.001730	-0.234288
C	1.087005	1.254364	0.160956

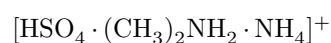
H	2.158746	1.272420	-0.031351
H	0.904429	1.271857	1.234240
H	0.610302	2.113260	-0.309059
C	1.082558	-1.256184	0.160699
H	2.153854	-1.279094	-0.033511
H	0.601103	-2.113282	-0.307757
H	0.901947	-1.272109	1.234339
N	-2.271376	0.001515	0.057159
H	-2.749068	-0.749907	-0.437570
H	-2.512063	-0.111269	1.040363



N	1.330701	-0.295503	-0.326201
H	1.489898	-0.970859	-1.071637
C	2.119495	0.917041	-0.644586
C	1.761214	-0.921993	0.945208
H	1.935855	1.679506	0.115221
H	3.194515	0.712717	-0.669548
H	1.817390	1.310308	-1.616857
H	1.562667	-0.237703	1.772520
H	2.830603	-1.156145	0.945683
H	1.202916	-1.844893	1.110872
N	-1.347901	0.281036	-0.341527
H	-1.495782	0.917217	-1.126530
H	-0.258006	0.045606	-0.330816
C	-2.121187	-0.973348	-0.589085
C	-1.726998	0.983060	0.922170
H	-2.785640	1.239942	0.900627
H	-1.129947	1.888687	1.019270
H	-1.528778	0.320046	1.763000
H	-3.186170	-0.749494	-0.640226
H	-1.791788	-1.415072	-1.528659
H	-1.932478	-1.667152	0.228939

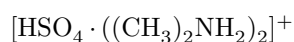


S	0.001296	-0.460925	-0.105845
O	0.000304	-1.455865	1.166249
O	0.003023	0.865666	0.536280
O	-1.229063	-0.729758	-0.856184
O	1.229183	-0.733662	-0.857889
H	0.001320	-2.373630	0.851157
N	-2.800901	1.193797	0.042578
H	-3.534741	0.922798	0.697384
H	-1.993453	1.587236	0.546855
H	-2.382307	0.340514	-0.443148
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



H	-1.565967	0.836299	-0.589150
S	0.849785	-0.500248	0.264168
O	-0.221611	-0.871030	1.181274
O	0.504409	0.632255	-0.618169
O	0.999287	-1.713589	-0.802161

O	2.164370	-0.337386	0.897942
H	-1.764697	-0.206156	0.602436
H	1.243456	-2.520633	-0.322610
N	-2.320649	0.366467	-0.068957
C	-3.075692	-0.536918	-0.988238
H	-3.587243	0.061258	-1.740748
H	-3.800662	-1.104816	-0.407461
H	-2.368759	-1.214044	-1.464544
C	-3.157504	1.363088	0.661073
H	-3.661504	2.007295	-0.057876
H	-2.511552	1.955183	1.307077
H	-3.893107	0.832434	1.263399
N	3.136662	1.658909	-0.515946
H	2.208532	1.726301	-0.962168
H	2.995093	0.850662	0.168149
H	3.854104	1.439357	-1.206569
H	3.371202	2.524165	-0.030395

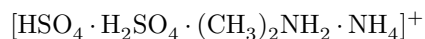


S	0.093795	-0.181845	-0.001433
O	-0.902850	0.888078	-0.001331
O	0.900018	-0.275985	-1.217770
O	0.900099	-0.275581	1.215024
N	3.354843	0.174368	-0.000146
H	2.706317	0.020580	-0.795594
H	2.702441	0.021126	0.792521
C	4.436799	-0.851108	0.002902
C	3.832061	1.588251	0.000420
H	5.051483	-0.725747	-0.887220
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

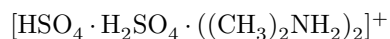


S	-1.087114	-1.366873	1.417527
O	-0.452215	-0.647491	2.492698
O	-2.294341	-0.808535	0.851623
N	2.067075	0.561518	2.591676
H	2.888414	-0.042648	2.628209
H	1.204382	0.002325	2.732892
N	-2.785095	1.601023	-0.624856
H	-3.553172	2.157369	-0.249914
H	-2.678147	0.724172	-0.083544
S	0.645168	1.673045	-0.817728

O	1.274362	2.067323	-2.233335
O	1.761481	1.557866	0.122133
O	-0.026480	0.399229	-1.126985
O	-0.325928	2.708787	-0.448116
H	1.783133	2.888611	-2.146825
O	-1.369808	-2.804352	1.994285
H	-1.879425	-3.340217	1.364116
H	2.140201	1.277778	3.314350
H	1.989130	1.009950	1.636851
H	-2.975468	1.367414	-1.599724
H	-1.869115	2.134234	-0.570474
O	-0.063760	-1.696779	0.292983
H	0.027819	-0.895344	-0.341672



S	-2.192333	-0.298221	-1.001468
O	-2.077121	1.107596	-0.694105
O	-1.624879	-0.772566	-2.239852
N	0.415947	-2.672622	-2.362314
H	1.037977	-2.216773	-1.638182
H	0.894853	-2.711879	-3.262048
C	0.127933	3.270055	1.390712
H	0.092351	2.368089	1.998022
H	-0.763519	3.874297	1.552285
H	1.019356	3.847307	1.630708
N	0.190823	2.859309	-0.044963
C	0.255655	3.992712	-1.013497
H	-0.625894	2.269076	-0.259258
H	1.017088	2.235509	-0.173664
H	0.300297	3.589179	-2.023621
H	-0.632140	4.613099	-0.900849
H	1.149307	4.580818	-0.811011
S	1.779064	-0.246604	0.345777
O	2.691949	-0.511886	1.635002
O	1.891273	-1.436440	-0.501506
O	2.243413	0.981979	-0.293250
O	0.444663	-0.074357	0.955781
H	3.615321	-0.620236	1.358923
O	-3.710017	-0.724940	-1.062170
H	-4.200039	-0.372766	-0.301146
H	0.170554	-3.617739	-2.067113
H	-0.440902	-2.089428	-2.440213
O	-1.687363	-1.160126	0.190994
H	-0.804091	-0.773947	0.565673

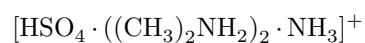


S	-1.007059	0.824322	0.753006
C	0.660146	-3.780141	0.782921
H	1.430736	-4.534111	0.935757
H	-0.325544	-4.216964	0.936288
H	0.740562	-3.361775	-0.218104
O	-1.062223	-0.520828	1.277928
O	-0.420115	1.857887	1.564547
N	0.865589	-2.672715	1.764387
C	0.793650	-3.087790	3.195498
H	1.788507	-2.225663	1.570304
H	0.169045	-1.934794	1.584960
H	-0.187793	-3.514180	3.397524
H	0.953600	-2.212532	3.822816

H	1.568555	-3.827605	3.389844
C	1.541275	3.983694	-0.724589
H	0.942383	3.327416	-1.353383
H	2.471261	4.237150	-1.230695
H	0.982963	4.889118	-0.491273
N	1.860278	3.260621	0.542482
C	2.670462	4.044651	1.520461
H	2.363749	2.378194	0.311313
H	0.982656	2.947364	0.985437
H	2.849664	3.427154	2.398811
H	3.619536	4.312221	1.058941
H	2.124783	4.944181	1.801550
S	2.872474	-0.531327	-0.142019
O	3.774703	-1.086866	-1.347730
O	1.508453	-0.825803	-0.637419
O	3.151946	0.896849	-0.014032
O	3.191694	-1.314088	1.049900
H	4.710175	-1.020174	-1.101416
O	-0.366762	0.819546	-0.666224
H	0.427657	0.146086	-0.713242
O	-2.466241	1.341085	0.429544
H	-2.971188	0.666549	-0.052755

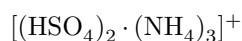


S	0.676339	0.093594	-0.166614
O	1.859729	0.709071	-0.804307
O	-0.152613	-0.671162	-1.103668
O	-0.118274	1.111659	0.579037
O	1.187528	-0.883712	0.946546
N	2.707572	-2.753750	-0.074670
H	2.207352	-3.279392	-0.787266
H	3.520433	-2.339804	-0.524358
H	1.793729	-1.635067	0.534430
H	3.046336	-3.419561	0.615003
N	-2.565438	-0.126259	0.009951
C	-3.657325	0.505819	-0.780836
C	-3.012695	-1.133056	1.014510
H	-4.336900	1.027741	-0.108267
H	-3.215778	1.208845	-1.485183
H	-4.197764	-0.267511	-1.324827
H	-1.847697	-0.551332	-0.619609
H	-1.978425	0.589908	0.472750
H	-3.682471	-0.657189	1.729565
H	-3.531148	-1.942000	0.501876
H	-2.133821	-1.519830	1.527636
N	1.857504	3.023075	0.388790
H	2.551541	3.188776	1.115758
H	2.103566	2.164380	-0.210867
H	0.957392	2.709894	0.796486
H	1.733914	3.859761	-0.178706

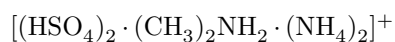


S	-0.014894	0.247385	0.259257
O	0.920264	-0.152715	1.323717
O	-0.461326	-0.903220	-0.548473
O	-1.132226	1.078540	0.730699
N	-3.129585	-0.650220	-0.064243
H	-2.240062	-1.039698	-0.447749
H	-2.754078	0.213708	0.371302

C	-4.078250	-0.320800	-1.163049
C	-3.672609	-1.555098	0.987519
H	-4.382312	-1.240004	-1.661883
H	-4.951887	0.180644	-0.748560
H	-3.575291	0.334188	-1.872449
H	-3.955357	-2.503493	0.532863
H	-4.543145	-1.090559	1.448720
H	-2.899452	-1.718294	1.736242
N	3.065065	-0.749295	-0.175423
H	2.822788	0.007287	-0.824079
H	2.338632	-0.617922	0.582846
C	4.441439	-0.558203	0.360867
C	2.822954	-2.063325	-0.844868
H	3.492826	-2.165375	-1.697755
H	1.782228	-2.090169	-1.163831
H	3.011315	-2.858622	-0.125339
H	5.163888	-0.624165	-0.451806
H	4.501156	0.419689	0.835927
H	4.641758	-1.334791	1.097325
O	0.846415	1.141263	-0.750827
H	0.693123	2.156963	-0.556329
N	0.345335	3.650285	-0.194950
H	0.022479	4.211766	-0.978084
H	1.070457	4.179443	0.281302
H	-0.432699	3.539467	0.451804

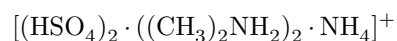


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O	1.560829	0.440145	-1.233462
N	-0.013134	-2.328094	-1.377575
H	0.904099	-2.147965	-0.902575
H	-0.739716	-2.280953	-0.640379
O	2.034699	-1.467053	0.217829
O	1.834018	0.773252	1.180012
N	-0.077755	2.569861	-1.101384
H	0.356263	3.438630	-0.793310
H	0.647667	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
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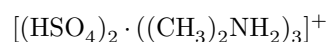
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O	-1.784207	0.560939	-1.150430
N	-0.158679	-1.903686	2.364280

H	-0.629043	-2.807663	2.370248
H	-0.830469	-1.162769	2.030855
O	-1.720674	0.007437	1.238621
O	-1.776304	-1.775141	-0.438496
N	0.159169	-1.904695	-2.363804
H	0.830787	-1.163447	-2.030808
H	-0.176630	-1.684606	-3.300048
C	-0.783984	3.258352	0.981869
H	-1.334671	2.569814	1.619301
H	-1.477802	3.900898	0.441577
H	-0.100653	3.864884	1.574549
N	-0.000232	2.454301	-0.000209
C	0.783756	3.258036	-0.982365
H	-0.649705	1.821631	-0.505820
H	0.649121	1.821517	0.505434
H	1.334197	2.569273	-1.619770
H	0.100606	3.864761	-1.575052
H	1.477813	3.900367	-0.442126
S	2.160246	-0.391627	0.102861
O	3.760963	-0.363174	-0.038560
O	1.720706	0.007257	-1.238748
O	1.783800	0.561304	1.150149
O	1.776599	-1.774945	0.438807
H	4.165963	-0.563245	0.818759
O	-3.760989	-0.363744	0.038769
H	-4.166026	-0.563613	-0.818580
H	0.629662	-2.808611	-2.368926
H	-0.644342	-1.920345	-1.683486
H	0.177309	-1.682792	3.300266
H	0.644696	-1.919737	1.683787

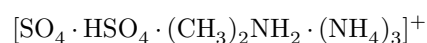


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O	1.912289	-0.289919	-1.009346
N	0.899027	2.334445	-1.086096
H	0.147501	2.221792	-0.373494
H	1.327981	1.389470	-1.154996
C	1.919256	3.297299	-0.583985
C	0.274158	2.702726	-2.388137
H	-0.191540	3.683079	-2.295217
H	-0.483858	1.957783	-2.623355
H	1.039740	2.727397	-3.162719
H	1.447291	4.264224	-0.414307
H	2.323653	2.905078	0.347164
H	2.713465	3.397739	-1.322915
O	1.071417	-1.762881	0.777817
O	2.074740	0.394268	1.328035
N	0.007399	-0.012400	3.111373
H	0.213575	-0.834134	3.677632
H	0.830994	0.197577	2.493178
C	-1.931776	-3.293493	-0.591499
H	-2.341522	-2.899201	0.336485
H	-1.465647	-4.262615	-0.417909
H	-2.720676	-3.390840	-1.336664
N	-0.903398	-2.334885	-1.086272
C	-0.272024	-2.705236	-2.384952
H	-0.154698	-2.225795	-0.370423
H	-1.327847	-1.387971	-1.156457
H	0.489217	-1.962071	-2.615793
H	0.190610	-3.686714	-2.288126

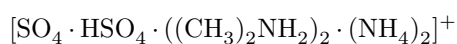
H	-1.033294	-2.728764	-3.163918
S	-2.037033	0.740094	0.390104
O	-3.440515	1.518236	0.519542
O	-2.068281	-0.391524	1.333648
O	-1.069253	1.765743	0.779133
O	-1.917738	0.292499	-1.004602
H	-4.160300	0.934933	0.236285
O	3.441262	-1.516650	0.509678
H	4.163098	-0.925662	0.248621
H	-0.823175	-0.200245	2.494942
H	-0.191039	0.784835	3.714236



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
H	0.298040	4.805860	-1.240080
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

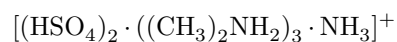


S	-3.281223	-0.320687	0.183762
O	-2.332063	-1.205606	0.876371
N	-0.969669	-1.952505	-1.657763
H	-1.925385	-1.533318	-1.716970
H	-0.282643	-1.131894	-1.580752
O	-3.259482	-0.503946	-1.272693
O	-3.168822	1.087562	0.577910
N	-0.346111	-0.170785	2.431664
H	-0.298775	-0.363601	3.428827
H	-1.219646	-0.554837	1.998978
N	-1.401935	2.519646	-0.989723
H	-1.547611	3.507256	-1.185200
H	-2.225078	2.093676	-0.509775
S	1.323016	0.610440	-0.307496
O	2.625382	1.144828	-0.764394
O	1.554849	-0.619576	0.542010
O	0.458073	0.255969	-1.478114
O	0.587608	1.625732	0.522630
H	3.831168	0.261623	-0.267908
O	-4.699474	-0.853777	0.723790
H	-5.407962	-0.321930	0.331087
H	-0.296269	0.834244	2.228592
H	0.469308	-0.555226	1.889385
H	-0.943924	-2.491881	-0.793048
H	-0.764712	-2.544835	-2.458945
H	-1.208612	2.003178	-1.849077
H	-0.559254	2.344001	-0.359555
C	5.208936	0.021092	1.312982
H	5.694301	-0.793476	1.850347
H	4.558380	0.577981	1.985119
H	5.962018	0.690887	0.900242
N	4.386099	-0.524096	0.201033
C	5.143555	-1.301840	-0.814601
H	3.601196	-1.075150	0.573429
H	5.623756	-2.159851	-0.344495
H	4.450711	-1.636872	-1.584699
H	5.898135	-0.656836	-1.262701



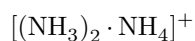
S	2.941102	-0.985477	-0.075658
O	2.674781	-0.413553	-1.377805
N	1.668978	2.311321	-0.115186
H	0.849911	1.769307	-0.501629
H	2.232634	1.601710	0.380975
C	1.154566	3.319442	0.852995
C	2.471288	2.876829	-1.235432
H	1.842258	3.549368	-1.817350
H	2.817304	2.050784	-1.852731
H	3.322468	3.423785	-0.830676
H	0.540931	4.041959	0.316427
H	0.541304	2.801340	1.587817
H	1.991674	3.826766	1.331743
O	2.059778	-2.146994	0.239358
O	2.948206	-0.028722	1.043546
N	0.717363	-1.217503	2.504952
H	1.147820	-1.778216	1.741409
H	1.478034	-0.688403	2.930284
C	-5.392434	-0.533404	1.121480
H	-4.729297	-0.472215	1.982784

H	-5.928935	-1.482073	1.129327
H	-6.102914	0.291700	1.151548
N	-4.575008	-0.424112	-0.114613
C	-5.346252	-0.468522	-1.383789
H	-3.823095	-1.131208	-0.120762
H	-3.961778	0.449020	-0.079522
H	-4.651264	-0.365563	-2.215443
H	-5.883019	-1.414101	-1.459531
H	-6.054554	0.358832	-1.398788
S	-1.421755	0.458007	0.060134
O	-1.825641	-0.992329	-0.154890
O	-0.418841	0.813871	-0.985699
O	-0.792127	0.593818	1.413556
O	-2.625841	1.315279	-0.024820
H	-0.745413	-1.672317	-1.210310
O	4.435828	-1.570078	-0.211986
H	4.740491	-1.882320	0.652446
H	0.021572	-0.511407	2.053454
H	0.261371	-1.808274	3.195940
N	0.123065	-1.885301	-1.783638
H	0.853811	-2.261899	-1.151112
H	0.469870	-0.975127	-2.103279
H	-0.053688	-2.509159	-2.566878

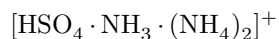


S	2.463601	0.551691	0.072081
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H	-0.419055	-0.555474	2.178328
H	1.129623	-1.033980	1.876834
C	0.034308	-2.406923	2.997680
C	0.907603	-0.175494	3.746538
H	0.121917	-0.064866	4.493057
H	1.192736	0.794894	3.344449
H	1.776985	-0.657109	4.192515
H	-0.745904	-2.375425	3.757232
H	-0.337157	-2.905395	2.105121
H	0.911442	-2.921699	3.388275
O	2.121978	0.704447	-1.351160
O	2.311702	-0.814598	0.567143
N	-5.403178	0.285013	-0.101371
H	-5.487906	0.905698	-0.901744
H	-4.032308	-0.577997	-0.113818
C	1.860121	-2.797983	-2.150356
H	2.374465	-2.752001	-1.192541
H	2.577312	-2.683514	-2.962392
H	1.331196	-3.744730	-2.253364
N	0.877420	-1.679993	-2.199392
C	0.110217	-1.572957	-3.470485
H	1.374709	-0.788457	-2.008955
H	0.198793	-1.771518	-1.407577
H	-0.609173	-0.763122	-3.363558
H	0.796071	-1.373635	-4.293107
H	-0.417462	-2.509520	-3.646800
S	-1.836835	-0.595546	-0.052396
O	-1.685913	0.325801	-1.201767
O	-1.722245	0.137304	1.228179
O	-0.904606	-1.733308	-0.114577
O	-3.252779	-1.253108	-0.132262
H	-0.901269	1.786704	-0.774096

O	4.052568	0.795737	0.212794
H	4.266823	1.687534	-0.097802
H	-5.513885	0.848077	0.737545
H	-6.191045	-0.357295	-0.136343
C	0.099662	3.430147	-1.589893
H	-0.736032	3.718556	-2.226666
H	0.798562	2.803275	-2.139979
H	0.610104	4.320995	-1.225061
N	-0.409506	2.646599	-0.431404
C	-1.328172	3.391239	0.471823
H	0.403071	2.292611	0.115598
H	-2.172420	3.765134	-0.107046
H	-1.679319	2.699620	1.235180
H	-0.794228	4.225873	0.924914



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
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H	0.892603	0.428764	-0.000132
H	-0.892622	0.428784	0.000127
H	0.000197	1.633687	0.825439
H	-0.000187	1.633697	-0.825431
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

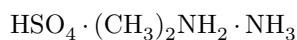


S	-0.009115	-0.004203	0.099276
O	0.214348	1.208862	0.911165
O	1.064800	-0.038573	-1.026342
O	0.115789	-1.244126	0.892421
O	-1.314344	0.052899	-0.612105
N	-1.638400	2.758208	-0.083680
H	-0.808407	2.352016	0.464307
H	-2.373219	3.095869	0.536004
H	-1.949190	1.923186	-0.610125
H	-1.344237	3.499920	-0.717431
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
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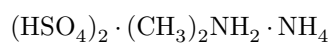


S	1.836243	0.241906	-0.181308
O	0.961415	0.627206	-1.313922
N	-0.189803	-2.109694	-1.546787
H	0.719948	-1.934475	-1.044417
H	-0.934417	-2.139156	-0.824954

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

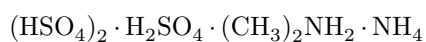


S	-0.393481	0.937791	-0.599382
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O	0.412330	0.049813	-1.440112
O	-1.802773	0.985110	-1.070902
O	-0.266432	0.733697	0.831748
H	0.356098	2.537423	-1.774347
N	-0.412938	-2.281757	0.587009
H	-0.511106	-2.939693	1.354183
H	0.475698	-2.469979	0.130554
H	-1.639070	-1.997395	-0.657913
H	-0.318692	-1.339838	0.979225
C	-1.764631	-2.005235	-2.745859
H	-1.737901	-3.092145	-2.837583
H	-0.763690	-1.585125	-2.829197
H	-2.405460	-1.586437	-3.522446
N	-2.293604	-1.625516	-1.412719
C	-3.681635	-2.059463	-1.142577
H	-2.212385	-0.569286	-1.313807
H	-3.746921	-3.147613	-1.186597
H	-3.969762	-1.715544	-0.149679
H	-4.353647	-1.623610	-1.882335

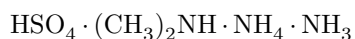


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O	-0.765034	-2.317697	2.513413
O	-0.109279	0.058822	2.372890
O	-2.087176	-0.684720	1.194262
N	-2.016535	1.952218	1.287707

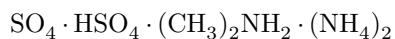
H	-2.883206	2.450479	1.103275
H	-1.738293	2.061410	2.261577
S	0.831410	1.910037	-0.936330
O	2.211997	1.593268	-0.546938
O	0.023095	0.721999	-1.223080
O	0.172877	2.872387	-0.050644
O	0.145438	-1.450740	0.440424
H	0.031802	-0.734165	-0.229521
H	1.495398	0.115095	2.106522
H	-2.126232	0.895007	1.138471
H	-1.234844	2.320126	0.688507
N	2.510750	0.227140	1.823107
C	3.154821	-1.111062	1.769812
C	3.164157	1.200833	2.731392
H	2.466272	0.647832	0.868793
H	3.148952	-1.551202	2.766792
H	2.573668	-1.736238	1.095133
H	4.179525	-1.008160	1.412242
H	3.125618	0.825381	3.753773
H	4.200419	1.348091	2.427243
H	2.628883	2.146643	2.663412
O	0.935602	2.734731	-2.330030
H	1.272841	2.126633	-3.002879



N	-3.615647	-5.002409	0.865570
H	-2.902888	-4.379682	0.430576
H	-3.249000	-5.633996	1.593619
H	-4.085121	-5.544224	0.143476
S	-3.028006	-1.749177	-0.319097
O	-2.216745	-2.966975	-0.365579
O	-2.903107	-1.013537	0.950897
O	-4.424492	-1.934572	-0.720083
H	-2.925970	-1.969471	2.371063
S	-4.550160	-2.705524	3.579042
O	-3.032070	-2.642900	3.095366
O	-4.502912	-3.366027	4.868395
O	-5.075151	-1.341707	3.576284
O	-5.262015	-3.538533	2.545680
H	-4.304965	-4.395047	1.361144
O	-2.447471	-0.769978	-1.470533
H	-1.491305	-0.691487	-1.340253
S	-4.838488	-6.720508	4.014828
O	-4.723972	-5.988976	5.403313
O	-6.063070	-5.992730	3.304813
O	-5.230471	-8.063316	4.260025
O	-3.643412	-6.437891	3.239777
H	-4.539561	-5.020679	5.269839
H	-5.829644	-5.049918	3.086578
H	-5.659109	-0.867205	2.053295
H	-5.479749	-1.146968	0.416996
N	-6.054076	-0.624795	1.114969
C	-5.873164	0.831263	0.876462
C	-7.458766	-1.106523	1.060699
H	-8.051012	-0.572601	1.803193
H	-7.865031	-0.935264	0.064202
H	-7.458465	-2.170363	1.290891
H	-6.241942	1.084002	-0.117212
H	-6.420377	1.391590	1.633884
H	-4.809260	1.050659	0.944587

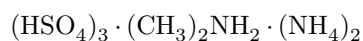


S	1.399007	-0.603519	0.000230
O	2.919816	-1.118453	-0.307625
O	1.446132	-0.019418	1.357584
O	0.546924	-1.787967	-0.075493
O	1.171209	0.392412	-1.041714
H	3.059697	-1.910726	0.228453
N	-0.827542	1.485888	1.401661
H	-1.250846	1.842315	2.253349
H	0.050520	0.945202	1.603978
H	-1.477204	0.798220	0.895351
H	-0.539257	2.268731	0.750598
N	0.363330	3.188636	-0.507559
H	-0.119422	3.601444	-1.299908
H	1.062123	3.858899	-0.200704
H	0.858374	2.356900	-0.845811
C	-3.413435	-1.132926	0.515487
H	-4.226311	-0.400208	0.520596
H	-3.238711	-1.457165	1.543975
H	-3.748751	-2.002943	-0.067192
N	-2.195736	-0.523980	-0.025578
C	-2.320505	-0.150788	-1.441345
H	-1.417645	-1.184285	0.048012
H	-3.032068	0.674282	-1.549156
H	-1.343226	0.166773	-1.806812
H	-2.670761	-0.985260	-2.064939

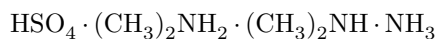


S	-2.241362	-0.408613	-0.019719
O	-3.636553	-0.701872	-0.164317
N	0.198638	-1.000940	2.706801
H	-0.727801	-0.689693	2.328783
H	0.417067	-1.920963	2.318788
O	-1.818982	0.130992	1.294228
O	-1.673199	0.453737	-1.109761
N	-0.004957	-1.069431	-2.684995
H	0.093910	-0.997603	-3.693331
H	-0.816884	-0.519823	-2.331091
S	2.092393	-0.636998	0.038320
O	3.451548	-1.089791	0.193438
O	1.723481	0.407150	1.107835
O	1.088573	-1.759219	0.179812
O	1.835279	0.034733	-1.294253
O	-1.480841	-1.819500	-0.180967
H	-0.487330	-1.717340	-0.025682
H	-0.545287	1.671148	-0.512471
H	0.918676	-0.347705	2.240627
H	0.228244	-0.999413	3.721756
H	-0.140960	-2.039935	-2.408810
H	0.871704	-0.657273	-2.139359
N	0.152416	2.281706	-0.033175
C	-0.555123	3.101456	0.982235
C	0.929923	3.065160	-1.026208
H	0.805208	1.593454	0.442742
H	-1.209166	3.815093	0.480261
H	-1.152453	2.431475	1.596931
H	0.176890	3.636195	1.587955
H	0.252667	3.678967	-1.621151

H	1.638141	3.704028	-0.498270
H	1.474956	2.360279	-1.649991

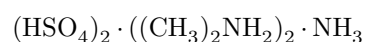


S	-3.681499	0.049504	0.245008
O	-3.568652	1.414648	-0.271151
O	-5.286923	-0.165568	0.294265
O	-3.159046	-0.967952	-0.675862
H	-5.453166	-1.067977	0.601488
S	1.942930	2.106100	0.061404
O	2.310772	1.109370	1.094906
O	2.821942	3.228905	-0.072583
O	2.052911	1.309771	-1.351088
S	0.233272	-1.801708	-0.524788
O	0.070279	-0.475851	-1.183909
O	0.309721	-1.653466	0.938980
O	1.360348	-2.556880	-1.060859
O	-1.059597	-2.630208	-0.884052
H	-1.864947	-2.060173	-0.745666
O	-3.197647	-0.106104	1.619164
N	-0.578161	0.669668	2.097838
N	-1.354315	1.801362	-1.766258
H	-2.286569	1.751345	-1.281573
H	-1.418631	2.281525	-2.659664
H	-0.660398	2.259636	-1.135508
H	-1.024157	0.829333	-1.882231
H	1.375844	0.585141	-1.343932
H	-1.611145	0.557146	2.035281
H	-0.233967	1.442926	1.490166
H	-0.159860	-0.217065	1.732189
H	-0.282370	0.830483	3.056718
O	0.492691	2.440652	0.199844
N	3.447003	-1.240697	0.306190
H	2.974576	-0.348315	0.604313
H	2.769069	-1.747290	-0.301716
C	4.663656	-0.883684	-0.470329
C	3.688718	-2.075399	1.512529
H	5.137838	-1.791066	-0.843506
H	4.361950	-0.244413	-1.298218
H	5.351208	-0.338700	0.175564
H	4.185653	-2.999879	1.219384
H	4.311615	-1.520586	2.213508
H	2.721884	-2.300769	1.958591

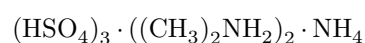


S	0.220973	-0.418896	-0.492254
O	1.463090	-0.451889	-1.480291
O	-0.730132	-1.399465	-1.005181
O	-0.333788	0.968472	-0.565734
O	0.727658	-0.713124	0.857816
H	2.267464	-0.023566	-1.023222
N	-2.054604	-1.562399	1.767169
H	-2.347721	-1.841234	2.698330
H	-2.099337	-2.380418	1.164871
H	-2.704225	-0.217136	0.784576
H	-1.058922	-1.321009	1.795296
C	-3.577703	0.062163	-1.096214
H	-4.560885	-0.314604	-0.808408
H	-2.965868	-0.731746	-1.520964

H	-3.691052	0.866518	-1.824001
N	-2.864095	0.577198	0.097385
C	-3.520234	1.714135	0.775087
H	-1.866406	0.842246	-0.196729
H	-4.510037	1.420320	1.128617
H	-2.906498	2.020176	1.621965
H	-3.615640	2.550026	0.081241
N	3.584697	0.566905	-0.183632
C	4.098826	-0.569637	0.593209
C	3.142716	1.684862	0.661844
H	4.300807	0.890964	-0.826680
H	3.275877	-0.985321	1.176398
H	4.456942	-1.342222	-0.090117
H	4.917003	-0.286278	1.271164
H	2.309621	1.341546	1.276281
H	3.942106	2.063095	1.315619
H	2.782964	2.497964	0.028953



S	-2.241362	-0.408613	-0.019719
O	-3.636553	-0.701872	-0.164317
N	0.198638	-1.000940	2.706801
H	-0.727801	-0.689693	2.328783
H	0.417067	-1.920963	2.318788
O	-1.818982	0.130992	1.294228
O	-1.673199	0.453737	-1.109761
N	-0.004957	-1.069431	-2.684995
H	0.093910	-0.997603	-3.693331
H	-0.816884	-0.519823	-2.331091
S	2.092393	-0.636998	0.038320
O	3.451548	-1.089791	0.193438
O	1.723481	0.407150	1.107835
O	1.088573	-1.759219	0.179812
O	1.835279	0.034733	-1.294253
O	-1.480841	-1.819500	-0.180967
H	-0.487330	-1.717340	-0.025682
H	-0.545287	1.671148	-0.512471
H	0.918676	-0.347705	2.240627
H	0.228244	-0.999413	3.721756
H	-0.140960	-2.039935	-2.408810
H	0.871704	-0.657273	-2.139359
N	0.152416	2.281706	-0.033175
C	-0.555123	3.101456	0.982235
C	0.929923	3.065160	-1.026208
H	0.805208	1.593454	0.442742
H	-1.209166	3.815093	0.480261
H	-1.152453	2.431475	1.596931
H	0.176890	3.636195	1.587955
H	0.252667	3.678967	-1.621151
H	1.638141	3.704028	-0.498270
H	1.474956	2.360279	-1.649991



S	-3.681499	0.049504	0.245008
O	-3.568652	1.414648	-0.271151
O	-5.286923	-0.165568	0.294265
O	-3.159046	-0.967952	-0.675862
H	-5.453166	-1.067977	0.601488
S	1.942930	2.106100	0.061404

O	2.310772	1.109370	1.094906
O	2.821942	3.228905	-0.072583
O	2.052911	1.309771	-1.351088
S	0.233272	-1.801708	-0.524788
O	0.070279	-0.475851	-1.183909
O	0.309721	-1.653466	0.938980
O	1.360348	-2.556880	-1.060859
O	-1.059597	-2.630208	-0.884052
H	-1.864947	-2.060173	-0.745666
O	-3.197647	-0.106104	1.619164
N	-0.578161	0.669668	2.097838
N	-1.354315	1.801362	-1.766258
H	-2.286569	1.751345	-1.281573
H	-1.418631	2.281525	-2.659664
H	-0.660398	2.259636	-1.135508
H	-1.024157	0.829333	-1.882231
H	1.375844	0.585141	-1.343932
H	-1.611145	0.557146	2.035281
H	-0.233967	1.442926	1.490166
H	-0.159860	-0.217065	1.732189
H	-0.282370	0.830483	3.056718
O	0.492691	2.440652	0.199844
N	3.447003	-1.240697	0.306190
H	2.974576	-0.348315	0.604313
H	2.769069	-1.747290	-0.301716
C	4.663656	-0.883684	-0.470329
C	3.688718	-2.075399	1.512529
H	5.137838	-1.791066	-0.843506
H	4.361950	-0.244413	-1.298218
H	5.351208	-0.338700	0.175564
H	4.185653	-2.999879	1.219384
H	4.311615	-1.520586	2.213508
H	2.721884	-2.300769	1.958591