

Supplementary Information

Nadykto, A. B., F. Yu, and J. Herb, Ammonia in positively charged atmospheric pre-nucleation clusters: A quantum-chemical study and atmospheric implications, Atmos. Chem. Phys., 2009.

Cartesian coordinates for the $(\text{H}_3\text{O}^+)(\text{NH}_3)(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_n$ ($n=0-5$) isomers.

$(\text{H}_3\text{O}^+)(\text{NH}_3)(\text{H}_2\text{SO}_4)$ -A 0.00 Kcal mole⁻¹

S	0.119368	0.124898	0.083527
O	1.270135	-0.830048	-0.506048
O	-0.701900	0.366960	-1.098373
O	-0.690374	-0.783989	1.030579
O	0.703621	1.231736	0.788209
H	-1.169302	-0.560664	-4.007935
H	1.992927	-0.922720	0.145858
O	-0.341322	-0.104959	3.429132
H	-0.567348	-0.491542	2.038560
H	-0.114892	0.835641	3.522610
H	-1.048241	-0.288102	4.069261
N	-0.371463	-0.016055	-3.663962
H	0.496639	-0.513773	-3.886915
H	-0.456152	0.119329	-2.589939
H	-0.364554	0.898247	-4.128187

$(\text{H}_3\text{O}^+)(\text{NH}_3)(\text{H}_2\text{SO}_4)$ -B 0.09 Kcal mole⁻¹

S	-0.564273	0.118917	0.093871
O	-0.969297	1.226337	0.910847
O	0.868269	-0.383543	0.397432
O	-1.414199	-1.178100	0.484488
O	-0.633490	0.264123	-1.360629
H	-2.314002	-0.901546	0.749986
H	0.423771	0.073843	-2.448537
O	1.565879	0.002079	2.791446
H	1.119329	-0.253446	1.411326
H	1.112675	0.738421	3.234666
H	1.581965	-0.735256	3.422735
N	1.111093	-0.018649	-3.285566
H	2.055230	-0.222774	-2.942195
H	1.127969	0.859017	-3.815592
H	0.806481	-0.777547	-3.904035

$(\text{H}_3\text{O}^+)(\text{NH}_3)(\text{H}_2\text{SO}_4)$ -C 0.22 Kcal mole⁻¹

S	0.244955	0.003236	0.023555
O	1.671790	0.077175	-0.686990
O	0.384745	-0.828667	1.221431

O	-0.269238	1.338012	0.214400
O	-0.548912	-0.851278	-0.977271
H	-1.019011	1.007243	3.310844
H	2.023827	0.984996	-0.602921
O	-0.734466	0.115944	-3.304323
H	-0.634874	-0.427790	-1.933653
H	-0.417654	-0.466220	-4.014392
H	-1.604013	0.443738	-3.586231
N	-0.666755	0.055506	3.461119
H	-0.230921	-0.311002	2.532294
H	-1.441937	-0.550305	3.749081
H	0.041241	0.069542	4.202290

(H₃O⁺)(NH₃)(H₂SO₄)-D 0.25 Kcal mole⁻¹

S	-0.577487	-0.120916	-0.091527
O	-1.391388	1.208968	-0.448739
O	0.869815	0.358822	-0.366157
O	-0.663669	-0.311408	1.356334
O	-0.998535	-1.191420	-0.948194
H	0.388601	-0.117868	2.451167
H	-2.298495	0.964373	-0.720941
O	1.583368	-0.002779	-2.757658
H	1.130191	0.244575	-1.380284
H	1.117378	-0.723447	-3.213270
H	1.629641	0.738307	-3.382947
N	1.135590	0.019776	3.228549
H	1.332444	-0.875617	3.687760
H	0.794969	0.687458	3.928138
H	1.999206	0.380982	2.810278

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₁-A 0.00 Kcal mole⁻¹

S	-0.500271	0.149873	-0.413947
O	-0.475344	-0.911423	-1.534962
O	0.826178	0.636513	-0.109253
O	-1.241201	1.409253	-1.051290
O	-1.329526	-0.388902	0.650452
H	-2.184195	1.201792	-1.208493
H	-0.904866	-0.713779	2.325790
O	1.318249	-0.614353	-3.295639
H	1.907866	0.155840	-3.262018
H	0.261159	-0.730135	-2.257645
H	1.063824	-0.730331	-4.225150
N	-0.425480	-0.757377	3.256047
H	0.517326	-0.254283	3.122766
H	-0.276901	-1.732345	3.529790
H	-0.994474	-0.289693	3.966304
O	1.838555	0.402888	2.512123

H	2.411607	1.083307	2.895634
H	1.686064	0.641498	1.572404

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₁-B 1.80 Kcal mole⁻¹

S	-0.170856	0.185026	0.039729
O	0.239578	1.323418	0.819235
O	0.986242	-0.376277	-0.852676
O	-0.488933	-1.027954	0.962943
O	-1.285538	0.373105	-0.900388
H	-0.903159	-0.701158	1.857303
H	-1.167657	0.061217	-2.350525
O	3.299480	-0.113890	0.195144
H	1.904765	-0.295191	-0.378705
H	3.408997	0.673401	0.752827
H	3.718551	-0.848161	0.671237
N	-1.100438	-0.154572	-3.428521
H	-0.150611	-0.472274	-3.645813
H	-1.306399	0.690750	-3.969506
H	-1.768691	-0.887914	-3.683800
O	-1.557766	-0.178676	3.122126
H	-1.192581	0.660912	3.445105
H	-1.650961	-0.757808	3.894791

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₁-C 2.04 Kcal mole⁻¹

S	-0.397858	0.135941	0.392799
O	-1.081951	1.239213	1.325220
O	-1.311260	-0.297644	-0.635637
O	0.895027	0.660762	-0.043406
O	-0.254789	-0.999509	1.416077
H	1.548696	0.438429	-1.654115
H	-1.034240	2.117393	0.898980
O	0.985808	-0.444016	3.548246
H	0.275333	-0.748294	2.285579
H	0.412875	-0.186745	4.289329
H	1.574544	-1.137059	3.889078
N	1.739808	0.236250	-2.666970
H	0.821803	-0.154857	-3.077544
H	2.497523	-0.446085	-2.750835
H	2.007949	1.096874	-3.151591
O	-0.694801	-0.533908	-3.352433
H	-1.153558	-0.585384	-2.486644
H	-1.068129	-1.222255	-3.922772

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₁-D 2.33 Kcal mole⁻¹

S	-0.416994	0.211106	0.392653
O	-1.061268	1.259239	1.411946
O	-1.362686	-0.135223	-0.640323

O	0.873345	0.745438	-0.040022
O	-0.267906	-0.993883	1.332215
H	1.478792	0.588646	-1.679938
H	-0.992293	2.165094	1.051667
O	1.066075	-0.624605	3.448363
H	1.664412	-1.346374	3.701694
H	0.300884	-0.817631	2.195590
H	0.527000	-0.431945	4.233175
N	1.653512	0.392562	-2.696899
H	1.813618	1.268292	-3.201064
H	0.772689	-0.109614	-3.066337
H	2.474832	-0.209262	-2.800088
O	-0.577686	-0.933202	-3.200417
H	-1.106653	-0.775527	-2.388895
H	-1.194954	-0.999419	-3.944059

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₁-E 2.68 Kcal mole⁻¹

S	-0.186636	-0.026164	-1.498362
O	-1.171787	-1.181621	-1.963956
O	1.129501	-0.552332	-1.256239
O	-0.032850	0.888398	-2.785848
O	-0.916893	0.680415	-0.473189
H	-0.862501	1.377468	-2.962532
H	-0.708976	-1.801888	-2.564214
O	-1.166050	-0.450876	4.279184
H	-0.469663	0.959665	1.382921
H	-0.803587	-1.227541	4.731985
H	-2.060239	-0.331809	4.633825
N	0.083904	0.972842	2.256776
H	1.022485	0.531902	2.025951
H	-0.405921	0.429122	3.010641
H	0.215711	1.940117	2.561720
O	2.290583	-0.326675	1.376266
H	2.168170	-0.492424	0.421027
H	3.243332	-0.234357	1.525283

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₁-F 5.60 Kcal mole⁻¹

S	-0.680586	-0.135905	0.509474
O	-1.394490	1.291403	0.552583
O	-0.863761	-0.610795	-0.836689
O	0.867889	0.229713	0.606769
O	-1.058504	-0.899711	1.666350
H	1.638172	0.117676	-1.144626
H	-1.714967	1.470640	1.458668
O	1.410997	0.094430	3.089229
H	1.171564	0.185834	1.602804
H	0.884235	-0.623017	3.480463

H	2.294308	0.044847	3.487292
N	1.916818	0.054226	-2.143860
H	2.548537	0.825209	-2.377263
H	1.025435	0.089295	-2.758955
H	2.400606	-0.834417	-2.303548
O	-0.339862	-0.072547	-3.520095
H	-1.019934	-0.210099	-2.834221
H	-0.734472	0.468996	-4.220353

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₂-A 0.00 Kcal mole⁻¹

S	-0.014583	-0.000263	0.231113
O	-0.613055	-1.078351	1.179342
O	1.028444	-0.667596	-0.525474
O	-1.078525	0.671973	-0.504186
O	0.597965	1.085598	1.165504
H	-1.216591	0.833971	-2.184629
H	-1.383274	-0.722695	1.765940
O	2.768757	0.297837	2.292766
H	3.343283	0.984661	2.666981
H	1.479363	0.761616	1.597451
H	3.342708	-0.271148	1.754971
N	-1.147655	0.776680	-3.235623
H	-2.020541	0.413038	-3.625189
H	-0.327393	0.108890	-3.434881
H	-0.961846	1.702453	-3.629101
O	1.007921	-0.764194	-3.297357
H	1.157633	-0.899288	-2.333264
H	1.221084	-1.597873	-3.741880
O	-2.568119	-0.293495	2.653855
H	-3.147102	-1.007589	2.965206
H	-2.367511	0.247235	3.434351

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₂-B 1.86 Kcal mole⁻¹

S	-0.047887	-0.112644	0.288557
O	0.723922	1.080845	0.924843
O	0.834290	-0.882228	-0.569520
O	-0.429034	-1.053188	1.466944
O	-1.256567	0.459920	-0.294386
H	-1.122344	-0.638581	2.108930
H	-1.486016	0.808435	-1.941830
O	3.201553	0.538064	1.321498
H	3.499494	-0.339966	1.034951
H	1.708027	0.831657	1.116899
H	3.608680	0.697517	2.187414
N	-1.480255	0.846234	-2.996122
H	-0.684034	0.190007	-3.303941
H	-1.301597	1.801625	-3.315329

H	-2.380212	0.529500	-3.364409
O	0.642442	-0.703342	-3.332617
H	0.819166	-1.489230	-3.870438
H	0.848632	-0.934048	-2.397588
O	-2.139412	-0.070873	3.113505
H	-3.061959	-0.350668	3.002868
H	-1.937420	-0.181171	4.056292

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₂-C 2.87 Kcal mole⁻¹

S	-0.467062	-0.375707	0.952669
O	-0.449712	-0.018912	2.462287
O	-1.024346	0.694523	0.160025
O	0.817274	-0.929763	0.557005
O	-1.578996	-1.508850	0.944572
H	1.189523	-0.172060	-3.174337
O	2.029631	-0.791093	-1.934889
H	-1.272160	-2.290610	1.445375
H	1.624452	-0.861291	-1.039040
H	2.727030	-1.460962	-1.978662
N	0.578963	0.320090	-3.900754
H	-0.313510	0.664425	-3.415603
H	0.341936	-0.326782	-4.656436
H	1.085188	1.117500	-4.293777
O	-1.505817	1.214730	-2.498938
H	-2.448547	1.289625	-2.705484
H	-1.433877	1.036627	-1.533307
O	1.484664	1.454832	3.212273
H	2.167736	1.030461	3.756202
H	0.361261	0.569431	2.742782
H	1.209647	2.250575	3.696186

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₂-D 7.19 Kcal mole⁻¹

S	-0.037926	0.080020	-1.788585
O	0.482680	1.332562	-2.615286
O	-1.074412	0.498577	-0.879828
O	-0.785585	-0.810567	-2.873193
O	1.152243	-0.589170	-1.340049
H	-0.133905	-1.270586	-3.440785
H	-0.041291	0.398901	3.527180
O	2.259522	-0.968299	1.287341
H	1.989719	-0.847754	0.355625
H	-0.263027	1.924094	-2.843631
H	3.164662	-1.312209	1.263620
N	-1.036499	0.070134	3.802469
H	-1.587077	-0.141220	2.917792
H	-1.510356	0.802497	4.336320

H	-0.977462	-0.772215	4.379607
O	-2.287835	-0.500639	1.468855
H	-3.230041	-0.648202	1.301181
H	-1.904878	-0.171822	0.628599
O	1.323797	0.871491	2.932490
H	1.789666	0.221850	2.327566
H	2.003027	1.373763	3.404368

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₂-E 8.54 Kcal mole⁻¹

S	-0.099274	0.046294	1.729036
O	-1.076248	1.123849	2.367079
O	1.033224	0.703875	1.132751
O	0.490052	-0.728879	2.983036
O	-0.958357	-0.827418	0.972930
H	-0.187389	-1.320686	3.369541
H	0.260647	0.375340	-3.379691
O	-1.564067	-1.188141	-1.790206
H	-1.458747	-1.103720	-0.819035
H	-0.562224	1.844574	2.785357
H	-2.217151	-1.893247	-1.919170
N	0.828237	-0.473431	-3.136482
H	1.578954	-0.233715	-2.425709
H	1.239331	-0.898110	-3.969743
H	0.137636	-1.114208	-2.698133
O	2.603001	0.005183	-1.139166
H	3.480464	0.414602	-1.162522
H	2.186089	0.288663	-0.300211
O	-1.174126	1.353458	-3.127305
H	-1.791021	0.715632	-2.720620
H	-1.703695	1.962787	-3.662199

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-A 0.00 Kcal mole⁻¹

S	0.000558	0.002488	-0.730488
O	0.496464	-1.147030	-1.658049
O	1.128793	0.538172	0.013798
O	-0.477804	1.141643	-1.679501
O	-1.141298	-0.525013	-0.001208
H	-1.421057	0.950944	-2.052095
H	-0.459560	-0.748630	3.552880
O	2.900366	-0.775816	-2.487484
H	3.376131	-0.059311	-2.037760
H	1.447588	-0.961553	-2.012819
H	3.075422	-0.666716	-3.435425
N	0.000162	-0.012503	4.183987
H	0.443898	0.738530	3.558901
H	0.722191	-0.444164	4.765529
H	-0.707135	0.405683	4.792864

O	1.180771	1.688224	2.494068
H	1.138088	2.654765	2.459984
H	1.160858	1.366891	1.559829
O	-2.863092	0.760539	-2.555809
H	-3.018048	0.631670	-3.504753
H	-3.352739	0.056710	-2.101018
O	-1.224154	-1.667825	2.481741
H	-1.195318	-1.345063	1.548171
H	-1.220753	-2.635198	2.445175

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-B 0.03 Kcal mole⁻¹

S	0.246820	-0.054885	-0.262551
O	0.371185	-0.927193	0.988805
O	-1.059182	0.589219	-0.308306
O	1.287100	1.101579	-0.093780
O	0.641874	-0.868979	-1.414587
H	2.245396	0.771831	-0.233871
H	-0.187491	-0.956390	-2.862680
O	-1.335915	-0.444731	2.674792
H	-1.923756	0.263070	2.366232
H	-0.380234	-0.675074	1.768795
H	-1.061659	-0.224254	3.612991
N	-0.822337	-0.863359	-3.704890
H	-1.520568	-0.082742	-3.454921
H	-1.316151	-1.742987	-3.873717
H	-0.276695	-0.617626	-4.533829
O	-2.441630	0.951295	-2.653597
H	-2.690211	1.849373	-2.917118
H	-2.035985	1.009123	-1.755345
O	3.744850	0.363610	-0.510243
H	4.436861	0.892949	-0.083440
H	3.982218	-0.563874	-0.352868
O	-0.766015	0.117203	5.199081
H	0.082560	0.449478	5.528736
H	-1.085189	-0.507237	5.868748

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-C 1.39 Kcal mole⁻¹

S	0.249399	-0.019225	0.254596
O	1.350519	-1.121335	0.407168
O	0.413366	0.977501	1.303615
O	0.528524	0.682102	-1.083740
O	-1.018923	-0.741937	0.195060
H	0.357689	0.075563	-1.964334
H	-2.072413	-0.960632	1.464102
O	3.474272	-0.089888	1.457135
H	3.331570	0.833083	1.721995
H	2.216580	-0.709633	0.776417

H	4.336342	-0.116346	1.013577
N	-2.671624	-0.902931	2.336169
H	-2.275495	-0.075536	2.897690
H	-2.600695	-1.769567	2.874523
H	-3.648616	-0.741076	2.082173
O	-1.297508	1.065306	3.463308
H	-1.546821	1.936642	3.804545
H	-0.623951	1.209095	2.756122
O	0.143030	-0.643734	-3.136925
H	-0.317394	-0.143624	-3.870107
H	0.940392	-1.042496	-3.516611
O	-1.189631	0.683149	-5.020265
H	-0.837306	1.433788	-5.521952
H	-1.778083	0.209556	-5.627699

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-D 1.95 Kcal mole⁻¹

S	0.033503	-0.142019	0.716626
O	0.513899	1.217596	1.315036
O	1.114557	-0.758806	-0.026267
O	-0.236159	-1.071798	1.936011
O	-1.221294	0.138574	0.034085
H	-1.065190	-0.798639	2.481321
H	-1.640124	0.926078	-1.430955
O	3.048176	1.153742	1.722133
H	3.454832	0.360785	1.336268
H	1.524718	1.180831	1.528084
H	3.425138	1.249931	2.610811
N	-1.898101	1.317212	-2.370710
H	-1.240605	0.871932	-3.128013
H	-1.796360	2.334634	-2.355706
H	-2.872998	1.086189	-2.577157
O	-2.302753	-0.464780	3.351290
H	-2.137242	-0.260954	4.285621
H	-3.010114	-1.129297	3.345756
O	1.323021	-1.428621	-2.739627
H	1.266488	-1.283439	-1.770144
H	1.326118	-2.388130	-2.871881
O	-0.352189	0.081617	-4.078297
H	0.307419	-0.525051	-3.613776
H	0.110515	0.486765	-4.826172

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-E 3.07 Kcal mole⁻¹

O	1.205681	-0.807673	-2.820487
H	1.886304	-0.125073	-2.707377
H	0.274062	-0.710065	-1.927378
H	0.876641	-0.757745	-3.772801
O	0.424000	-0.695714	-5.323207

H	-0.460604	-0.385494	-5.571287
H	0.604360	-1.464244	-5.886759
S	-0.591858	0.509639	-0.249367
O	-1.297874	1.570469	-1.226156
O	0.751473	1.002810	0.044485
O	-1.468658	0.282461	0.883243
O	-0.562806	-0.704545	-1.154606
H	-0.082067	-0.990854	3.891822
H	-1.433363	2.411725	-0.748488
O	-1.461089	-1.243898	3.135648
H	-1.539420	-0.769435	2.273558
H	-1.964864	-2.066471	3.055758
N	0.842004	-0.667744	4.335971
H	1.374591	-0.073862	3.620797
H	1.408924	-1.476623	4.600583
H	0.642611	-0.116047	5.173712
O	2.115257	0.691857	2.407319
H	2.710796	1.448228	2.509527
H	1.629867	0.829816	1.556488

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-F 3.34 Kcal mole⁻¹

S	-0.508660	0.130838	0.371439
O	0.000064	1.500946	1.144717
O	0.765291	-0.527369	0.068145
O	-1.323087	-0.606213	1.348636
O	-1.278942	0.620754	-0.770966
H	-0.724987	-1.197891	2.724811
H	-0.736786	2.141396	1.138698
O	-1.557380	0.044357	-3.324439
H	-2.199286	-0.662927	-3.491351
H	-1.532963	0.213439	-2.338598
H	-0.305565	-0.143481	-3.801292
N	-0.255535	-1.407565	3.663705
H	-0.952867	-1.436394	4.411266
H	0.425149	-0.606076	3.821642
H	0.237247	-2.302346	3.624448
O	1.180432	0.867161	3.688393
H	0.975808	1.250318	2.809792
H	2.091347	1.116873	3.902514
O	0.737963	-0.262385	-4.132274
H	1.404056	-0.292244	-3.265666
H	0.985108	0.473670	-4.716796
O	2.194244	-0.312006	-2.146136
H	1.667830	-0.365596	-1.291817
H	2.844523	-1.031157	-2.125212

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-G 3.50 Kcal mole⁻¹

S	0.213038	-0.260333	0.306389
O	-1.116734	-0.966475	0.481517
O	0.057584	1.168451	0.064228
O	0.876391	-0.439482	1.746057
O	1.025789	-0.997076	-0.656519
H	1.783146	0.033593	1.784110
H	0.592538	-1.597302	-2.171005
O	-2.698371	0.026910	2.022030
H	-2.993428	0.927730	1.810736
H	-1.899990	-0.426233	1.179723
H	-2.149002	0.061773	2.882122
N	0.341548	-1.877967	-3.155583
H	-0.070410	-1.003091	-3.663883
H	-0.341916	-2.637966	-3.129326
H	1.180383	-2.202667	-3.642288
O	-0.547823	2.233360	-2.439777
H	-0.032479	3.038801	-2.593730
H	-0.297472	1.915011	-1.542116
O	-0.994006	-0.008632	3.956989
H	-1.084339	-0.634313	4.692447
H	-0.212038	-0.290430	3.440825
O	-0.500145	0.343424	-4.267414
H	-0.526661	1.102584	-3.603472
H	-1.272781	0.441768	-4.842471
O	3.185988	0.733156	1.861743
H	3.954830	0.224055	2.162247
H	3.260798	1.608704	2.272104

$(\text{H}_3\text{O}^+)(\text{NH}_3)(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_3\text{-H}$ 4.14 Kcal mole⁻¹

S	-0.537950	-0.507696	-0.165968
O	-0.783522	-1.285941	1.032726
O	-1.152349	0.910737	-0.051101
O	1.013504	-0.271620	-0.316986
O	-0.995031	-1.054796	-1.429847
H	1.526921	-0.288037	0.617942
H	-0.908368	-0.447112	-2.988203
O	-0.902349	1.917775	2.244988
H	-1.070146	1.326116	0.920785
H	-1.662003	2.409602	2.593238
H	-0.666872	1.223611	2.908448
N	-0.587566	-0.020527	-3.899757
H	-1.242769	0.703061	-4.205616
H	-0.514131	-0.742095	-4.620946
H	0.366562	0.402866	-3.681471
O	2.239757	-0.230984	1.871638
H	1.599892	-0.319663	2.623451
H	2.922191	-0.908623	1.997607

O	0.014232	-0.365765	3.458388
H	-0.140996	-0.758270	4.331639
H	-0.435522	-0.933182	2.789037
O	1.653421	0.986956	-2.844480
H	1.672319	0.629950	-1.932386
H	2.571778	1.117705	-3.122348

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-I 5.54 Kcal mole⁻¹

S	-0.420079	0.204483	-1.247072
O	-0.911490	-0.584696	-2.486966
O	0.993692	-0.007987	-1.029347
O	-0.522561	1.741721	-1.668960
O	-1.369991	-0.052727	-0.187718
H	-1.461513	2.011198	-1.713142
H	0.699739	0.020485	3.919394
O	0.706097	-0.539188	-4.458004
H	0.342808	-0.819619	-5.313329
H	-0.229523	-0.570525	-3.271564
H	1.551610	-1.004403	-4.354771
N	1.196447	-0.703312	3.348446
H	1.776536	-0.250832	2.580048
H	0.419190	-1.242780	2.912325
H	1.777645	-1.305471	3.933836
O	2.572040	0.308425	1.250209
H	3.106956	1.115085	1.221054
H	2.067304	0.277879	0.407241
O	-1.367848	-1.217394	2.333279
H	-1.973314	-1.973697	2.362247
H	-1.428661	-0.863445	1.416421
O	-0.798998	0.920306	4.211535
H	-1.457073	0.369788	3.745693
H	-1.253097	1.340115	4.956355

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₃-H 10.22 Kcal mole⁻¹

S	-0.151485	-0.110484	-2.100917
O	-1.391659	-1.015397	-2.507649
O	0.873870	-0.921698	-1.501685
O	0.453437	0.361776	-3.490497
O	-0.729400	1.017279	-1.414631
H	-0.122517	1.037090	-3.903793
H	0.970799	0.013326	3.241828
O	0.016990	-0.966890	4.100433
H	0.221113	-1.882647	4.338751
H	-1.084880	-1.880705	-2.847971
H	-0.867869	-0.970592	3.640844
N	1.398009	0.778854	2.623377
H	2.005892	0.363137	1.869935

H	1.942442	1.430545	3.191857
H	0.608889	1.281960	2.170159
O	2.818602	-0.193558	0.477754
H	3.661974	-0.666689	0.427168
H	2.273961	-0.518150	-0.266153
O	-1.046836	1.657633	1.312534
H	-1.440718	2.540916	1.390669
H	-0.999706	1.474929	0.347695
O	-2.174827	-0.631362	2.593765
H	-2.014389	0.228358	2.149254
H	-3.078718	-0.597968	2.940602

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-A 0.00 Kcal mole⁻¹

S	0.000000	0.000000	0.000000
O	0.000000	1.567632	0.000000
O	0.000000	-0.486851	1.371568
O	-1.302344	-0.450734	-0.659052
O	1.140051	-0.373064	-0.845723
H	-1.261490	-0.527619	-1.757540
H	2.507123	0.524648	-0.595740
O	-0.741004	2.669024	2.150991
H	-0.258173	2.168547	2.852511
H	-0.409067	1.984233	0.871623
H	-1.673560	2.705229	2.413641
N	3.350151	1.145782	-0.404673
H	3.381700	1.387563	0.640158
H	3.261000	2.002190	-0.956900
H	4.207991	0.659213	-0.676022
O	0.985785	0.934963	3.407989
H	0.975877	0.517961	4.283610
H	0.655132	0.255241	2.760642
O	-1.273746	-0.637703	-3.106938
H	-0.597169	-1.258066	-3.420563
H	-2.148136	-0.936085	-3.498278
O	3.370316	1.616441	2.236661
H	3.801076	2.359123	2.684236
H	2.546803	1.408343	2.750859
O	-3.538764	-1.435161	-4.222640
H	-4.225966	-1.916479	-3.737021
H	-4.007485	-0.837328	-4.825071

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-B 0.07 Kcal mole⁻¹

S	0.029107	-0.324029	1.368138
O	0.459951	1.072076	0.835669
O	0.753087	-1.379992	0.681470
O	0.483396	-0.387319	2.851871
O	-1.428980	-0.350729	1.305488

H	-0.106142	0.180153	3.478944
H	-2.165491	-0.319209	-0.240830
O	2.617356	1.147937	-0.448545
H	2.595270	0.344733	-1.028713
H	1.416471	1.082484	0.383676
H	3.471438	1.150695	0.010390
N	-2.566260	-0.309582	-1.215354
H	-1.752125	-0.367027	-1.950220
H	-3.101898	0.551086	-1.349986
H	-3.193905	-1.108815	-1.330981
O	1.849672	-1.116496	-1.760090
H	2.379686	-1.849596	-2.109838
H	1.484677	-1.416706	-0.888427
O	-0.933301	1.013461	4.477251
H	-0.441748	1.403089	5.217908
H	-1.690964	0.553069	4.872081
O	-0.626274	-0.530209	-2.963207
H	-0.564867	0.089849	-3.732430
H	0.287479	-0.719481	-2.648483
O	-0.699321	1.160533	-5.091675
H	-0.758177	0.779133	-5.981099
H	-0.166281	1.963974	-5.190574

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-C 0.64 Kcal mole⁻¹

S	-0.280199	-0.269729	-0.276379
O	-0.548137	1.129945	0.375848
O	-0.745087	-1.324595	0.611479
O	-1.130362	-0.340563	-1.548402
O	1.143038	-0.261368	-0.619712
H	-0.766769	0.242555	-2.391345
H	2.180141	0.268630	0.534637
O	-2.242686	1.150978	2.253490
H	-1.988765	0.376115	2.810965
H	-1.328093	1.116723	1.076539
H	-3.195132	1.083206	2.085835
N	2.819007	0.626713	1.309013
H	2.370979	0.415611	2.259370
H	2.945432	1.635521	1.197919
H	3.730195	0.166501	1.244493
O	-0.378936	0.958193	-3.508027
H	-1.092493	1.501173	-3.876701
H	-0.026198	0.391008	-4.253142
O	-0.883955	-1.022573	3.262571
H	-0.822410	-1.318781	2.314515
H	-1.181855	-1.788599	3.777519
O	1.649465	-0.039495	3.634204
H	0.726210	-0.403619	3.602821

H	1.738707	0.426791	4.477925
O	0.642094	-0.581194	-5.419844
H	0.159328	-1.302528	-5.850889
H	1.257379	-0.236243	-6.084337

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-D 1.97 Kcal mole⁻¹

S	0.213038	-0.260333	0.306389
O	-1.116734	-0.966475	0.481517
O	0.057584	1.168451	0.064228
O	0.876391	-0.439482	1.746057
O	1.025789	-0.997076	-0.656519
H	1.783146	0.033593	1.784110
H	0.592538	-1.597302	-2.171005
O	-2.698371	0.026910	2.022030
H	-2.993428	0.927730	1.810736
H	-1.899990	-0.426233	1.179723
H	-2.149002	0.061773	2.882122
N	0.341548	-1.877967	-3.155583
H	-0.070410	-1.003091	-3.663883
H	-0.341916	-2.637966	-3.129326
H	1.180383	-2.202667	-3.642288
O	-0.547823	2.233360	-2.439777
H	-0.032479	3.038801	-2.593730
H	-0.297472	1.915011	-1.542116
O	-0.994006	-0.008632	3.956989
H	-1.084339	-0.634313	4.692447
H	-0.212038	-0.290430	3.440825
O	-0.500145	0.343424	-4.267414
H	-0.526661	1.102584	-3.603472
H	-1.272781	0.441768	-4.842471
O	3.185988	0.733156	1.861743
H	3.954830	0.224055	2.162247
H	3.260798	1.608704	2.272104

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-E 2.30 Kcal mole⁻¹

S	0.000000	0.000000	0.000000
O	0.000000	1.463170	0.000000
O	0.000000	-0.567548	1.386491
O	-1.367131	-0.499928	-0.660335
O	1.041687	-0.602366	-0.829331
H	-2.174922	0.071996	-0.349671
H	1.261592	-2.123448	-1.335706
O	0.216911	0.809546	3.389600
H	0.135078	0.222390	2.454207
H	1.138706	1.081755	3.531846
H	-0.412410	1.674738	3.378462
N	1.195810	-3.124498	-1.694486

H	1.794608	-3.744067	-1.144615
H	1.473059	-3.167224	-2.677912
H	0.167045	-3.384180	-1.583804
O	-3.370768	0.913631	0.110102
H	-3.068654	1.838499	0.284284
H	-4.116110	0.972807	-0.506946
O	-1.895221	3.136160	0.769448
H	-1.891046	4.013728	0.356017
H	-1.120952	2.629237	0.391700
O	-1.460112	-3.239371	-1.384910
H	-1.620063	-2.328977	-1.049952
H	-2.040407	-3.831412	-0.884087
O	-1.230563	2.831749	3.352308
H	-1.565782	3.043313	2.434840
H	-1.990918	2.829410	3.953689

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-F 2.33 Kcal mole⁻¹

S	-0.346489	0.494310	0.455545
O	-0.168739	1.369938	-0.703127
O	-1.123163	-0.741790	0.118866
O	1.093735	-0.024763	0.915635
O	-0.883083	1.162773	1.639155
H	1.692058	-0.266002	0.103288
H	-0.995742	0.684305	3.180881
O	-2.163899	-1.109253	-2.057735
H	-1.687079	-0.895059	-1.081352
H	-2.987603	-0.601214	-2.144005
H	-1.517781	-0.882321	-2.879781
N	-0.878029	0.285636	4.161886
H	-1.744042	-0.156440	4.477090
H	-0.615759	1.026391	4.816323
H	-0.091264	-0.428975	4.070261
O	2.577429	-0.625416	-1.095522
H	2.343887	-0.041431	-1.857990
H	3.534229	-0.544752	-0.962191
O	1.254676	0.976223	-2.894431
H	1.568512	1.770585	-3.354370
H	0.727041	1.283519	-2.103013
O	1.208480	-1.242736	3.473023
H	1.284254	-0.989356	2.526072
H	1.371714	-2.196016	3.524949
O	-0.667518	-0.560145	-3.966988
H	0.112602	-0.000192	-3.689916
H	-0.328352	-1.310104	-4.479173

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-G 2.37 Kcal mole⁻¹

S	-0.641277	-0.413212	-0.257982
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O	-1.064745	-1.072507	-1.479949
O	0.923952	-0.503533	-0.146227
O	-0.957182	1.107154	-0.307570
O	-1.177065	-0.904929	0.994077
H	-0.781678	1.528925	-1.257764
H	-1.550290	-0.421683	2.584034
O	2.105998	-0.704978	-2.344551
H	1.407400	-0.625075	-1.091168
H	2.612560	-1.520043	-2.485760
H	1.456990	-0.629201	-3.089719
N	-1.644912	-0.212642	3.607599
H	-0.649844	0.014538	3.997635
H	-2.043043	-1.026751	4.081709
H	-2.267691	0.587351	3.742419
O	-0.466619	2.117928	-2.575714
H	-0.400113	1.414380	-3.266676
H	-1.077121	2.794192	-2.907163
O	2.310296	0.457529	2.200613
H	1.879032	0.164893	1.371806
H	2.791802	1.269218	1.981635
O	0.780307	0.446946	4.360299
H	1.400298	0.460052	3.569952
H	1.270894	0.056264	5.098248
O	-0.109809	-0.272745	-3.885572
H	-0.371916	-0.594072	-4.762234
H	-0.663536	-0.740023	-3.215681

$(\text{H}_3\text{O}^+)(\text{NH}_3)(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_4\text{-H}$ 3.51 Kcal mole⁻¹

S	0.509829	0.402607	-0.513069
O	1.690139	-0.670938	-0.465182
O	0.663515	1.084396	-1.781709
O	-0.773377	-0.397654	-0.465598
O	0.639954	1.232995	0.698645
H	-1.294033	-1.014001	-1.977412
H	1.931614	-0.848430	0.483542
O	-1.405512	2.048204	2.330302
H	-1.821537	0.620725	2.116266
H	-0.682020	2.135803	1.669115
H	-2.013736	2.793039	2.207954
N	-1.519458	-1.319568	-2.965541
H	-1.417898	-2.333755	-3.048602
H	-0.828621	-0.809683	-3.625020
H	-2.480284	-1.059215	-3.201167
O	0.163413	0.204104	-4.313280
H	0.569180	0.650796	-3.534356
H	0.875559	0.008130	-4.939926
O	2.063127	-0.511896	2.275079

H	2.948460	-0.439272	2.666418
H	1.771718	0.398678	2.044312
O	-0.228135	-1.693600	3.265473
H	0.676918	-1.330829	3.105095
H	-0.328268	-1.830003	4.219610
O	-1.896914	-0.390940	1.873485
H	-1.264390	-0.925689	2.509605
H	-1.493386	-0.458410	0.934736

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-I 3.83 Kcal mole⁻¹

S	-0.236846	-0.120169	-0.049847
O	-0.802250	-1.126151	-0.960576
O	0.464820	0.982251	-0.715659
O	-1.579619	0.558214	0.649389
O	0.481552	-0.654763	1.102184
H	-2.343638	0.350688	0.081090
H	1.302228	-0.209648	4.061083
O	0.296047	1.974415	-3.126586
H	0.336077	1.627862	-2.179793
H	0.985518	2.651276	-3.211885
H	0.385322	0.958815	-4.013921
N	0.479516	-0.349896	4.746133
H	0.644944	0.177633	5.606155
H	0.383161	-1.341013	4.980094
H	-0.417735	-0.010468	4.275201
O	2.298236	0.154646	2.882986
H	1.786240	-0.085543	2.068331
H	3.193182	-0.197944	2.771822
O	-0.069050	-1.917669	-3.349972
H	0.610914	-2.607148	-3.305125
H	-0.306616	-1.659202	-2.407653
O	-1.773789	0.415169	3.468807
H	-1.706261	0.464926	2.488107
H	-2.335569	1.157151	3.737257
O	0.424848	0.082969	-4.685077
H	0.225569	-0.831991	-4.109290
H	-0.236780	0.173929	-5.390823

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₄-J 16.59 Kcal mole⁻¹

S	0.293546	-0.054736	2.181433
O	0.928524	-0.318089	0.882040
O	-0.448571	1.332751	2.082740
O	-0.866895	-1.123726	2.323510
O	1.058908	-0.059396	3.379022
H	-1.237405	-1.314911	1.417271
H	0.289857	-1.431227	-2.871911
O	-1.730860	1.380447	-0.304500

H	-0.912858	1.418631	1.194443
H	-2.463328	2.016714	-0.325086
H	-1.106538	1.608152	-1.073603
N	0.577571	-1.682623	-1.905747
H	0.943225	-2.637806	-1.875253
H	-0.250013	-1.600138	-1.266610
H	1.324161	-1.000890	-1.608703
O	-0.161016	-0.338354	-4.380514
H	-1.002920	-0.467891	-4.848023
H	0.494859	-0.219334	-5.087948
O	2.239545	0.455803	-1.204360
H	3.191431	0.637168	-1.243276
H	1.989455	0.375779	-0.245313
O	-1.774701	-1.293710	-0.293700
H	-2.620461	-1.753543	-0.418106
H	-1.961324	-0.311952	-0.357020
O	-0.014859	1.777597	-2.229290
H	-0.145566	1.300462	-3.069425
H	0.887089	1.528330	-1.923716

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-A 0.00 Kcal mole⁻¹

O	3.123698	0.462803	1.270103
H	3.305303	-0.319095	0.724857
H	1.748757	0.754697	1.166537
H	3.504816	0.284088	2.173645
O	4.278682	-0.012705	3.642501
H	3.791904	-0.202213	4.458732
H	4.999761	0.582345	3.899300
S	-0.001864	-0.004128	0.099553
O	-0.708201	-1.015356	1.027979
O	1.012488	-0.728927	-0.666404
O	-1.023671	0.721264	-0.656310
O	0.712774	1.007439	1.021342
H	-0.261677	0.840820	-4.105914
O	-0.762337	1.923458	-3.050103
H	-0.827227	1.564716	-2.125742
H	-0.434353	2.831113	-2.975289
N	-0.009864	0.007096	-4.739007
H	0.246956	-0.830735	-4.113559
H	0.785069	0.242806	-5.337167
H	-0.809822	-0.224730	-5.331984
O	0.753972	-1.918479	-3.065886
H	0.434966	-2.829799	-2.997336
H	0.815933	-1.565180	-2.139326
O	-3.116271	-0.462854	1.286252
H	-3.289441	0.321829	0.742056
H	-1.743430	-0.761569	1.179443

H	-3.494461	-0.280861	2.190385
O	-4.259834	0.020616	3.662721
H	-3.767125	0.186513	4.480520
H	-4.997459	-0.556442	3.913492

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-B 0.65 Kcal mole⁻¹

S	0.017139	-0.372116	0.601594
O	1.563047	-0.530675	0.789058
O	-0.492172	-1.367402	-0.332913
O	-0.507979	-0.727865	1.986554
O	-0.272003	1.021476	0.250543
H	-0.089091	-0.139193	2.813170
H	-0.638504	1.667595	-1.253802
O	2.877621	0.381999	-1.215410
H	2.419485	0.296782	-2.088692
H	2.084783	-0.160711	-0.028342
H	3.761169	-0.002442	-1.319100
N	-0.798525	1.969221	-2.252877
H	0.033881	1.682325	-2.802655
H	-0.940435	2.979193	-2.308605
H	-1.627397	1.438374	-2.651172
O	0.387076	0.549218	3.887538
H	1.317204	0.343459	4.070117
H	-0.117982	0.393700	4.739044
O	-0.579163	-1.601838	-2.976462
H	-0.540063	-1.617754	-1.979063
H	-0.542568	-2.525236	-3.270178
O	1.261630	0.319277	-3.446505
H	0.675749	-0.488717	-3.422010
H	1.634845	0.366948	-4.340273
O	-0.889682	0.174777	6.183987
H	-1.480901	-0.578837	6.332968
H	-1.311314	0.932897	6.616858
O	-2.568055	0.287362	-3.425447
H	-3.496116	0.088861	-3.232313
H	-2.069851	-0.558553	-3.338857

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-C 0.67 Kcal mole⁻¹

S	-0.103829	-0.140496	-0.003763
O	-0.625197	1.249107	0.508210
O	-0.211154	-1.131796	1.076754
O	-0.881687	-0.526970	-1.196578
O	1.330616	0.139584	-0.325834
H	-0.710588	0.065357	-2.547603
H	2.206174	-0.188086	1.075057
O	-2.677162	1.172588	2.020502
H	-2.471182	0.465456	2.677997

H	-1.516454	1.182943	1.036332
H	-3.571214	1.003864	1.686998
N	2.686897	-0.466298	1.981129
H	2.072915	-0.204420	2.822607
H	3.600523	-0.012855	2.053884
H	2.819672	-1.480890	1.976622
O	-1.381563	-0.805140	3.429398
H	-1.753554	-1.590570	3.859655
H	-1.035548	-1.091979	2.538773
O	-0.669423	-1.190488	-5.402824
H	0.058777	-1.745666	-5.721090
H	-1.173711	-0.927381	-6.188300
O	1.142374	0.009330	4.129519
H	1.155448	0.808702	4.676101
H	0.188110	-0.236155	4.007885
O	1.834274	1.262703	-2.751816
H	2.017172	2.214228	-2.713773
H	1.772598	0.941330	-1.812001
O	-0.463687	0.518449	-3.453721
H	-0.492708	-0.152997	-4.213410
H	0.507425	0.882189	-3.292305

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-D 1.35 Kcal mole⁻¹

S	0.495907	0.099261	-0.157030
O	0.603424	1.384164	-0.851894
O	-0.911131	-0.296563	0.136280
O	0.961956	-1.042981	-1.190503
O	1.368653	-0.022283	1.015014
H	1.909503	-0.849184	-1.513812
H	1.373500	0.702146	2.511711
O	-2.442525	0.094385	-1.923177
H	-1.958790	-0.065812	-1.036222
H	-2.156715	1.078673	-2.175815
H	-1.953719	-0.556463	-2.564486
N	1.355456	1.032694	3.515937
H	0.515913	0.548307	4.020549
H	1.242698	2.048612	3.544734
H	2.237497	0.785483	3.969868
O	-0.777660	-0.099161	4.546390
H	-0.785741	-0.630690	5.355813
H	-1.217317	-0.651730	3.826926
O	-0.933502	-1.446384	-3.278128
H	-1.173913	-2.348511	-3.539568
H	-0.188956	-1.516925	-2.639451
O	3.344444	-0.623924	-2.160349
H	3.624322	0.297946	-2.274219
H	4.101478	-1.087199	-1.769082

O	-1.528741	2.410927	-2.217894
H	-1.365369	2.849145	-3.066663
H	-0.650950	2.232943	-1.794757
O	-1.779249	-1.478648	2.537247
H	-2.740439	-1.576971	2.468128
H	-1.481052	-1.113054	1.673372

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-E 1.44 Kcal mole⁻¹

S	-0.339198	-0.159183	0.289349
O	-0.460894	-1.206437	-0.745481
O	0.985859	-0.212693	0.978387
O	-0.331768	1.241897	-0.431070
O	-1.466957	-0.176752	1.232663
H	-1.214689	1.388039	-1.066834
H	-1.533434	-0.138134	2.858450
O	2.936189	-0.189456	-0.759807
H	2.270595	-0.232159	0.010237
H	2.578810	-0.923925	-1.428773
H	2.744616	0.742577	-1.183535
N	-1.393998	-0.129553	3.913632
H	-0.331293	-0.085572	4.046766
H	-1.783138	-0.977601	4.331144
H	-1.843117	0.689930	4.328466
O	1.236115	0.128379	3.709476
H	1.994688	-0.314258	4.117330
H	1.302173	-0.011607	2.733714
O	2.108220	2.012490	-1.695623
H	2.509146	2.880169	-1.534742
H	1.217383	2.015545	-1.281449
O	-2.240305	1.569757	-1.963195
H	-2.544614	0.649160	-2.252163
H	-3.012606	2.040071	-1.614494
O	-2.614199	-0.946971	-2.537519
H	-3.424611	-1.471995	-2.463915
H	-1.984935	-1.294872	-1.869116
O	1.765275	-1.837036	-2.242689
H	0.884444	-1.796987	-1.794228
H	2.015468	-2.770011	-2.323013

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-F 2.84 Kcal mole⁻¹

S	-0.059248	-0.046820	-0.221517
O	0.102220	-0.996662	-1.355354
O	1.263979	0.212206	0.454826
O	-0.428867	1.347704	-0.801718
O	-1.067602	-0.503231	0.731072
H	-1.208866	1.302019	-1.545571
H	-1.104322	0.062051	4.082697

O	3.037792	0.957895	-1.156707
H	2.306617	0.732395	-0.426150
H	2.729177	0.299683	-2.035794
H	2.965890	1.898411	-1.394211
N	-0.284900	-0.220447	4.728143
H	0.582540	-0.358917	4.116685
H	-0.503000	-1.091346	5.217252
H	-0.116435	0.515017	5.418023
O	1.744028	-0.636172	3.028947
H	2.697498	-0.578620	3.184058
H	1.587790	-0.353572	2.093102
O	-2.096873	0.563243	2.960814
H	-1.789311	0.228355	2.076047
H	-3.056765	0.440255	2.989455
O	-2.154072	1.249152	-2.593370
H	-2.318731	0.283803	-2.825516
H	-3.011767	1.662523	-2.415229
O	-2.137256	-1.345797	-3.026661
H	-2.839988	-1.993926	-2.871943
H	-1.432392	-1.531248	-2.370412
O	2.165716	-0.492106	-2.902595
H	1.337664	-0.799792	-2.409831
H	2.684132	-1.274695	-3.149415

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-G 2.92 Kcal mole⁻¹

S	0.506567	-0.200967	0.117820
O	-0.332443	-1.389080	-0.059024
O	-0.293874	1.051583	0.259246
O	1.257054	-0.398645	1.516996
O	1.563381	-0.059699	-0.900725
H	2.201483	0.002453	1.451102
H	1.223536	-0.968423	-2.301942
O	-2.086315	0.780194	2.140664
H	-1.440704	1.015561	1.386987
H	-2.483894	-0.149301	1.839169
H	-1.464359	0.590481	2.948864
N	0.840123	-1.450453	-3.159640
H	0.098938	-0.787387	-3.601069
H	0.407051	-2.329729	-2.867469
H	1.589177	-1.644904	-3.827446
O	-1.355053	2.052219	-2.151990
H	-1.128071	2.984510	-2.285485
H	-0.941053	1.789290	-1.298884
O	-0.353806	0.127097	3.883343
H	-0.025393	0.701309	4.592075
H	0.402158	-0.071548	3.292342
O	-0.833684	0.346297	-4.101208

H	-1.059649	1.028446	-3.396302
H	-1.633484	0.203340	-4.627332
O	3.597274	0.670218	1.276859
H	3.720345	0.768570	0.317581
H	4.384803	0.206770	1.603381
O	-2.710495	-1.507952	1.319589
H	-1.936437	-1.646552	0.718595
H	-3.516695	-1.702101	0.818183

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-H 3.84 Kcal mole⁻¹

S	0.000000	0.000000	0.000000
O	0.000000	1.455014	0.000000
O	0.000000	-0.623649	1.345346
O	-1.502577	-0.451996	-0.540103
O	0.953389	-0.610039	-0.922538
H	-1.689458	0.038337	-1.363007
H	1.846268	-2.030459	-1.070941
O	-1.217964	0.736559	3.248375
H	-0.678864	0.192236	2.588617
H	-1.278088	1.696750	2.815016
H	-2.163427	0.282692	3.301165
N	2.385301	-2.926210	-1.199768
H	1.861294	-3.729826	-0.676755
H	3.330539	-2.809161	-0.827528
H	2.448790	-3.139960	-2.198058
O	-0.597967	-3.388195	1.667253
H	-1.555279	-3.308362	1.490915
H	-0.282798	-2.460064	1.636905
O	-3.457181	-0.423802	3.245358
H	-3.753580	-0.860653	4.058351
H	-3.460843	-1.104312	2.522006
O	0.931569	-4.740416	0.018878
H	0.303962	-4.295693	0.673822
H	1.252754	-5.552904	0.436330
O	-3.179179	-2.103391	1.096230
H	-2.738213	-1.540877	0.422633
H	-3.973920	-2.461178	0.669747
O	-1.269023	2.893489	1.965975
H	-0.769067	2.594493	1.167846
H	-0.832752	3.693278	2.298182

(H₃O⁺)(NH₃)(H₂SO₄)(H₂O)₅-I 5.38 Kcal mole⁻¹

S	0.697084	0.076667	-0.923646
O	1.381517	0.555705	-2.146178
O	-0.426723	-0.840318	-1.240161
O	1.810313	-0.830399	-0.157071
O	0.398021	1.089277	0.064588

H	2.250208	-1.425624	-0.793043
H	-1.869429	1.011573	2.565909
O	-1.654295	-0.644144	-3.616495
H	-1.323438	-0.833000	-2.692192
H	-0.628257	0.032015	-4.169556
H	-1.884171	-1.489356	-4.034747
N	-1.924779	0.077004	3.052766
H	-2.000150	-0.668285	2.316933
H	-2.745684	0.050589	3.659796
H	-1.039693	-0.075842	3.619451
O	-2.026590	-1.737624	0.942190
H	-1.965954	-2.701565	1.010032
H	-1.459755	-1.481683	0.182123
O	-1.667287	2.327346	1.491808
H	-0.925784	2.073685	0.903491
H	-1.497768	3.241109	1.764194
O	0.440165	-0.200856	4.354318
H	1.238230	-0.257585	3.761253
H	0.629939	-0.763050	5.118850
O	2.561926	-0.360597	2.693720
H	3.241484	0.324626	2.781201
H	2.360586	-0.411528	1.741415
O	0.308860	0.579198	-4.402425
H	0.804325	0.629598	-3.472349
H	0.128156	1.477911	-4.728146