

Supplementary Information

CH₃NH₂- A 0.000 kcal/mol

C	-0.000001	-0.014117	-0.711750
N	0.000000	0.124148	0.754286
H	-0.000110	0.973055	-1.195372
H	0.882411	-0.557268	-1.074197
H	-0.882293	-0.557465	-1.074196
H	-0.815235	-0.321328	1.167132
H	0.815234	-0.321331	1.167130

(CH₃NH₂)(H₂O)- A 0.00 kcal/mol

C	-0.488627	-0.014010	-1.564840
N	0.634791	0.036070	-0.618205
H	-1.043062	0.929899	-1.515019
H	-0.196396	-0.185986	-2.612931
H	-1.174868	-0.812671	-1.262493
H	1.172252	-0.830179	-0.653674
H	1.280404	0.786603	-0.862099
O	-0.141344	-0.104673	2.127025
H	-0.517893	0.733343	2.429375
H	0.098543	0.047940	1.177113

(CH₃NH₂)(H₂O)- B 0.06 kcal/mol

C	-0.554830	-0.000173	1.424006
N	0.708637	0.000158	0.669326
H	-1.139117	0.882208	1.141248
H	-1.139464	-0.881882	1.139873
H	-0.431648	-0.001035	2.518386
H	1.268716	0.817662	0.909991
H	1.268522	-0.817772	0.908988
O	-0.262745	0.000323	-2.008792
H	0.457939	-0.002719	-2.653747
H	0.185535	0.000885	-1.123721

(CH₃NH₂)(H₂O)- C 1.03 kcal/mol

C	-0.524444	0.014242	-1.496769
N	0.673361	0.002523	-0.642942
H	-1.211305	-0.768827	-1.157856
H	-1.040029	0.973493	-1.377279
H	-0.322231	-0.139178	-2.568535
H	1.173078	-0.881430	-0.739672
H	1.324217	0.734557	-0.926436
O	-0.199719	-0.099363	2.072066
H	-0.044121	0.743059	2.521024
H	0.151273	0.030119	1.153437

(CH₃NH₂)(H₂O)₂- A 0.00 kcal/mol

C	-0.182126	-0.391002	2.119926
N	-0.082656	0.567868	1.011255
H	-0.161529	-1.408615	1.714052
H	0.686130	-0.281762	2.779884
H	-1.093811	-0.283470	2.728421

H	-0.873036	0.463745	0.365854
H	-0.101967	1.525861	1.359210
O	1.459707	-0.188632	-1.125583
H	2.064149	0.492408	-1.453437
H	1.088978	0.165244	-0.257458
O	-1.223054	0.011506	-1.757555
H	-0.243090	-0.125956	-1.756104
H	-1.587691	-0.759512	-2.213669

(CH₃NH₂)(H₂O)₂- B 0.01 kcal/mol

C	-0.182641	-0.390784	-2.118879
N	-0.083234	0.568168	-1.010184
H	0.683284	-0.278406	-2.781375
H	-0.157293	-1.408499	-1.713504
H	-1.096471	-0.286201	-2.724650
H	-0.107241	1.526061	-1.358084
H	-0.871220	0.460974	-0.362243
O	1.460618	-0.188349	1.123503
H	2.069803	0.489233	1.449446
H	1.089135	0.166251	0.256001
O	-1.222921	0.012038	1.758846
H	-0.243272	-0.125720	1.758647
H	-1.589819	-0.765676	2.201525

(CH₃NH₂)(H₂O)₂- C 0.01 kcal/mol

C	-0.181650	-0.390379	2.119352
N	-0.082191	0.567713	1.009938
H	-0.155380	-1.408405	1.714850
H	0.683749	-0.276875	2.782318
H	-1.095926	-0.285895	2.724441
H	-0.870075	0.459894	0.361925
H	-0.106566	1.525854	1.357120
O	1.459616	-0.188430	-1.125741
H	2.069830	0.488387	-1.451346
H	1.089697	0.165932	-0.257510
O	-1.224065	0.012151	-1.756803
H	-1.590346	-0.766041	-2.199132
H	-0.244162	-0.124337	-1.757988

(CH₃NH₂)(H₂O)₂- D 0.12 kcal/mol

C	-0.195345	-0.391574	2.104828
N	0.005823	0.574354	1.016246
H	-0.328510	-1.390782	1.675071
H	0.695319	-0.418617	2.743462
H	-1.068432	-0.177876	2.740980
H	-0.801482	0.579073	0.383561
H	0.108818	1.518756	1.386108
O	1.449993	-0.013326	-1.240428
H	1.963956	-0.830930	-1.179569
H	1.116408	0.177424	-0.308557
O	-1.282293	-0.146430	-1.638495
H	-0.297000	-0.163739	-1.724538

H	-1.599368	0.313703	-2.427816
(CH ₃ NH ₂)(H ₂ O) ₂ - E 0.13 kcal/mol			
C	-0.194323	-0.390261	2.106525
N	0.004646	0.572979	1.015446
H	-0.324574	-1.391080	1.679602
H	0.696136	-0.413108	2.745617
H	-1.068239	-0.177257	2.741831
H	-0.802012	0.574383	0.381938
H	0.106598	1.518710	1.382065
O	1.449813	-0.012771	-1.240891
H	1.965719	-0.829229	-1.180828
H	1.115352	0.175991	-0.308790
O	-1.282124	-0.147178	-1.638674
H	-1.600275	0.315180	-2.426299
H	-0.296811	-0.163289	-1.725885
(CH ₃ NH ₂)(H ₂ O) ₃ - A 0.00 kcal/mol			
C	0.131410	0.461307	-2.525302
N	0.022008	-0.503108	-1.422338
H	-0.736975	0.372275	-3.189025
H	0.132556	1.477482	-2.113944
H	1.041308	0.342569	-3.133938
H	0.032537	-1.457301	-1.782411
H	0.826957	-0.411780	-0.783346
O	-1.921874	-0.174091	0.430959
H	-2.520946	0.544248	0.183211
H	-1.261133	-0.279866	-0.343635
O	-0.177371	0.322791	2.404901
H	-0.325946	-0.337735	3.096467
H	-0.900619	0.163353	1.729054
O	1.961888	-0.174687	0.797532
H	2.621201	0.522961	0.916020
H	1.247398	0.025609	1.462586
(CH ₃ NH ₂)(H ₂ O) ₃ - B 0.02 kcal/mol			
C	0.132957	0.463870	-2.520101
N	0.022259	-0.504081	-1.420531
H	-0.734297	0.376615	-3.185590
H	0.132838	1.478830	-2.105631
H	1.043881	0.347662	-3.127753
H	0.031045	-1.457144	-1.783529
H	0.826903	-0.415681	-0.780670
O	-0.177883	0.325607	2.399612
H	-0.324703	-0.330189	3.095983
H	-0.903435	0.163699	1.726861
O	-1.923440	-0.176211	0.429215
H	-1.262108	-0.281656	-0.345200
H	-2.524770	0.540088	0.181191
O	1.963714	-0.177732	0.798406
H	2.616251	0.527203	0.911057
H	1.245707	0.022612	1.459744

(CH₃NH₂)(H₂O)₃- C 0.02 kcal/mol

C	0.132175	0.467812	-2.517042
N	0.018951	-0.505545	-1.422400
H	-0.735225	0.386169	-3.183010
H	0.134612	1.480549	-2.097264
H	1.042863	0.352345	-3.125125
H	0.026831	-1.456690	-1.790447
H	0.823663	-0.421481	-0.781961
O	-1.922981	-0.178734	0.432624
H	-2.524810	0.536909	0.183940
H	-1.263435	-0.285365	-0.342912
O	-0.174358	0.329281	2.398826
H	-0.320222	-0.323208	3.098496
H	-0.900964	0.164177	1.727989
O	1.963398	-0.181555	0.794854
H	2.614782	0.525469	0.900930
H	1.247717	0.021137	1.457983

(CH₃NH₂)(H₂O)₃- D 0.03 kcal/mol

C	0.132397	0.469608	2.514642
N	0.018943	-0.506715	1.422701
H	0.133854	1.481262	2.092204
H	-0.734453	0.389204	3.181501
H	1.043615	0.356377	3.122382
H	0.823547	-0.424373	0.781911
H	0.026456	-1.456871	1.793273
O	-1.922794	-0.179547	-0.431843
H	-1.263504	-0.286889	0.343886
H	-2.525047	0.535681	-0.183044
O	1.963201	-0.182439	-0.794399
H	1.247857	0.020688	-1.457675
H	2.614724	0.524599	-0.899446
O	-0.174479	0.330267	-2.398196
H	-0.900670	0.164310	-1.727238
H	-0.320780	-0.320873	-3.099012

(CH₃NH₂)(H₂O)₃- E 0.14 kcal/mol

C	0.139975	0.539837	-2.442496
N	0.030640	-0.528074	-1.436929
H	-0.723053	0.506001	-3.117634
H	0.125487	1.509835	-1.933770
H	1.057412	0.487590	-3.048525
H	0.052520	-1.442717	-1.887643
H	0.830354	-0.490526	-0.786097
O	-0.191999	0.205204	2.401283
H	-0.312371	1.090269	2.773639
H	-0.912241	0.108770	1.710135
O	-1.922516	-0.069792	0.374451
H	-1.258033	-0.306536	-0.367823
H	-2.537992	-0.814095	0.433940
O	1.963644	-0.077617	0.765157

H	2.589590	-0.694215	1.169265
H	1.240958	0.040767	1.440856
(CH ₃ NH ₂)(H ₂ O) ₃ - F 0.14 kcal/mol			
C	0.140173	0.539068	2.444165
N	0.030973	-0.526998	1.436674
H	0.125133	1.510040	1.937281
H	-0.722645	0.503653	3.119514
H	1.057797	0.486088	3.049878
H	0.830821	-0.488568	0.786081
H	0.052525	-1.442468	1.885736
O	-1.922587	-0.070215	-0.374638
H	-2.537822	-0.814806	-0.432986
H	-1.258175	-0.305264	0.368261
O	1.963430	-0.078075	-0.766089
H	1.240584	0.039080	-1.441806
H	2.591365	-0.692382	-1.170584
O	-0.192421	0.205727	-2.401867
H	-0.312577	1.091840	-2.771793
H	-0.912231	0.107870	-1.710539
(CH ₃ NH ₂)(H ₂ O) ₃ - G 0.15 kcal/mol			
C	0.140697	0.539510	2.442511
N	0.031706	-0.527605	1.436219
H	0.124589	1.509995	1.934683
H	-0.721693	0.504139	3.118440
H	1.058729	0.487913	3.047778
H	0.831076	-0.489398	0.785021
H	0.053457	-1.442710	1.885989
O	-1.923113	-0.070205	-0.373321
H	-2.538746	-0.814450	-0.432133
H	-1.258203	-0.306282	0.368875
O	-0.193267	0.205643	-2.400464
H	-0.312826	1.091518	-2.771191
H	-0.913461	0.108428	-1.709372
O	1.964037	-0.077681	-0.766761
H	2.589756	-0.694406	-1.171065
H	1.239950	0.039382	-1.441247
(CH ₃ NH ₂)(H ₂ O) ₄ - A 0.00 kcal/mol			
C	0.155239	0.678675	2.820256
N	0.110613	-0.455058	1.883954
H	0.044583	1.611494	2.256134
H	-0.683397	0.617403	3.523568
H	1.089408	0.739014	3.399926
H	0.901420	-0.397171	1.220863
H	0.222770	-1.332543	2.392447
O	-2.126740	-0.307162	0.402293
H	-2.629649	-1.128797	0.493270
H	-1.283211	-0.422159	0.981802
O	-1.526290	0.240583	-2.124126
H	-1.921341	1.105303	-2.303709

H	-1.766480	0.030362	-1.169260
O	1.120223	0.155757	-2.486948
H	1.266981	-0.555452	-3.126402
H	0.125620	0.199036	-2.367027
O	2.288805	-0.287899	-0.091317
H	1.880712	-0.128506	-0.988255
H	2.998869	0.365136	-0.021787

(CH₃NH₂)(H₂O)₄- B 0.01 kcal/mol

C	0.154998	0.680373	-2.818924
N	0.109540	-0.455110	-1.884839
H	-0.684017	0.621381	-3.522007
H	0.045600	1.612227	-2.252935
H	1.088991	0.740891	-3.398907
H	0.220712	-1.331760	-2.394983
H	0.900370	-0.399115	-1.221629
O	-2.126990	-0.308521	-0.401352
H	-1.284142	-0.422643	-0.981901
H	-2.629664	-1.130305	-0.492277
O	-1.525632	0.241311	2.124790
H	-1.921457	1.105629	2.304609
H	-1.766186	0.030610	1.170230
O	2.288326	-0.289269	0.089932
H	1.881069	-0.128898	0.987029
H	2.999169	0.362812	0.019364
O	1.121504	0.156147	2.486345
H	0.126970	0.200016	2.366824
H	1.268151	-0.554654	3.126282

(CH₃NH₂)(H₂O)₄- C 0.15 kcal/mol

C	0.131993	0.549701	-2.914782
N	-0.031321	-0.467699	-1.865340
H	-0.743569	0.552358	-3.575393
H	0.202593	1.537717	-2.446120
H	1.030455	0.407389	-3.534242
H	-0.083428	-1.396983	-2.283447
H	0.793730	-0.463230	-1.242936
O	-2.173966	-0.168326	-0.268542
H	-2.694422	0.582025	-0.588216
H	-1.368192	-0.254396	-0.904521
O	1.242392	0.185927	2.424608
H	1.441261	1.054577	2.801613
H	0.241343	0.141557	2.382985
O	2.263692	-0.184604	-0.048444
H	2.962533	-0.845424	0.053362
H	1.910186	-0.040991	0.874004
O	-1.423176	0.088173	2.264258
H	-1.815757	-0.665403	2.727030
H	-1.720980	-0.002872	1.306918

(CH₃NH₂)(H₂O)₄- D 0.45 kcal/mol

C	-0.241926	1.214075	2.424082
---	-----------	----------	----------

N	0.099584	-0.178989	2.757278
H	0.552494	1.634411	1.797500
H	-1.164737	1.223262	1.833372
H	-0.379274	1.868127	3.298851
H	0.968078	-0.218918	3.290393
H	-0.622312	-0.595401	3.345108
O	-0.156550	0.880595	-2.690007
H	0.680386	0.611656	-2.204243
H	-0.174678	1.847516	-2.659875
O	1.897576	0.016166	-1.213476
H	2.526522	-0.559044	-1.671715
H	1.355015	-0.596772	-0.611553
O	-1.902775	-0.436403	-1.095555
H	-1.349679	0.090877	-1.738370
H	-2.428946	-1.034842	-1.644560
O	0.300249	-1.461365	0.262906
H	0.238050	-1.075046	1.181579
H	-0.554438	-1.219297	-0.172872

(CH₃NH₂)(H₂O)₄- E 0.88 kcal/mol

C	0.024693	1.183440	2.128803
N	-0.099682	-0.264734	1.888426
H	0.122819	1.694924	1.164914
H	-0.881472	1.559038	2.618041
H	0.894457	1.454039	2.745796
H	0.742455	-0.603755	1.396504
H	-0.151555	-0.762863	2.777184
O	2.253098	-0.878230	0.198057
H	2.417999	-1.771378	-0.134621
H	1.960471	-0.357492	-0.598928
O	-1.299243	0.119408	-2.159803
H	-1.656799	-0.185317	-1.268206
H	-1.827167	0.897379	-2.389058
O	-2.176643	-0.627411	0.229702
H	-2.480340	-1.545223	0.269556
H	-1.396511	-0.553618	0.899952
O	1.314365	0.628598	-1.859875
H	1.732981	0.537973	-2.727050
H	0.339655	0.449874	-2.010526

(CH₃NH₂)(H₂O)₄- F 2.38 kcal/mol

C	-0.855704	-0.672805	-2.309074
N	-0.054645	0.473843	-1.851788
H	-0.311578	-1.224915	-3.084979
H	-1.020465	-1.349771	-1.463045
H	-1.839431	-0.390941	-2.714047
H	0.080423	1.142063	-2.610369
H	-0.553305	0.964405	-1.090986
O	2.179685	-0.166130	-0.520615
H	2.441645	-1.071180	-0.742013
H	1.358507	0.048179	-1.110178
O	1.113789	0.176535	1.865813

H	1.790858	0.280403	2.548041
H	1.602241	0.010989	0.996413
O	-1.271263	1.481226	0.673810
H	-1.606928	0.610725	0.981159
H	-0.419701	1.526018	1.147599
O	-1.268177	-1.183527	1.673681
H	-0.366684	-0.847091	1.903941
H	-1.671108	-1.443796	2.513911

(CH₃NH₂)(H₂O)₄- G 2.85 kcal/mol

C	2.202245	0.614425	-1.329445
N	1.057834	-0.084390	-0.731996
H	1.913119	1.038486	-2.298009
H	2.504886	1.441454	-0.676651
H	3.078186	-0.032455	-1.487168
H	0.738145	-0.847616	-1.332699
H	1.297990	-0.481125	0.187966
O	-1.275984	0.998022	-0.303471
H	-1.346565	1.930466	-0.554208
H	-0.278667	0.690219	-0.490991
O	-1.240810	0.395078	2.338521
H	-2.006840	-0.159180	2.544737
H	-1.358625	0.666061	1.385689
O	1.131666	-0.962574	2.108757
H	1.730549	-0.691602	2.818169
H	0.276734	-0.491475	2.294662
O	-1.515615	-0.970859	-2.316618
H	-2.278378	-1.563220	-2.263978
H	-1.682904	-0.273177	-1.644394

(CH₃NH₂)(H₂O)₄- H 3.29 kcal/mol

C	1.697968	-0.088870	-1.763299
N	1.430288	0.679219	-0.532638
H	0.937331	-0.870012	-1.869523
H	1.612301	0.570304	-2.634428
H	2.694712	-0.553668	-1.776818
H	1.564198	0.089994	0.304753
H	2.083257	1.458370	-0.448334
O	1.343020	-0.753503	2.060270
H	1.405435	-1.711791	2.177133
H	0.385443	-0.535177	2.211549
O	-1.281593	0.009900	2.231577
H	-1.345341	0.497931	1.366028
H	-1.471980	0.665965	2.916771
O	-1.727983	-0.990989	-2.047168
H	-2.364113	-1.601927	-1.649571
H	-1.645961	-0.258916	-1.395379
O	-1.146402	1.107579	-0.242009
H	-1.442770	1.986656	-0.516994
H	-0.108673	1.057067	-0.398280

(CH₃NH₂)(H₂O)₅- A 0.00 kcal/mol

C	-1.246312	-0.804896	-2.766968
N	-0.624744	-0.196714	-1.581457
H	-1.891932	-1.635465	-2.459230
H	-1.879368	-0.064142	-3.268981
H	-0.518512	-1.184480	-3.500222
H	-0.008637	-0.867327	-1.113462
H	0.008942	0.563717	-1.853215
O	-2.366085	0.526638	0.308883
H	-2.661982	1.432005	0.138304
H	-1.697174	0.293135	-0.447037
O	-1.288250	0.224293	2.694684
H	-1.833965	-0.437452	3.142230
H	-1.709308	0.350172	1.784433
O	1.289164	-0.368465	2.563757
H	1.728327	0.376040	2.998450
H	0.304947	-0.161821	2.620686
O	1.999624	-0.811982	0.038458
H	1.761698	-0.640353	0.999096
H	2.709292	-1.468754	0.055050
O	1.998044	1.296955	-1.734709
H	2.134813	0.599596	-1.046941
H	2.343969	2.111987	-1.345737

(CH₃NH₂)(H₂O)₅- B 0.45 kcal/mol

C	1.902026	-0.819181	-1.198500
N	1.511789	0.471776	-0.599017
H	1.336163	-1.619207	-0.708658
H	1.640096	-0.829355	-2.262056
H	2.973270	-1.040881	-1.086856
H	1.679614	0.458535	0.421164
H	2.079830	1.223873	-0.990021
O	1.724163	0.369603	2.322811
H	0.818430	0.095900	2.638111
H	2.337051	-0.225699	2.776277
O	-0.761938	-0.384748	3.089595
H	-1.379043	-0.357076	2.303018
H	-1.164952	0.200757	3.746235
O	-0.570398	-0.216754	-3.684821
H	-1.359094	-0.604502	-4.088482
H	-0.871495	0.125344	-2.812186
O	-2.386774	-0.251336	0.955193
H	-1.905463	0.130268	0.163504
H	-2.763494	-1.090232	0.654674
O	-1.029453	0.813929	-1.098860
H	-1.228954	1.759292	-1.170011
H	0.008570	0.740083	-0.871948

(CH₃NH₂)(H₂O)₅- C 0.52 kcal/mol

C	1.902889	-0.815922	-1.207599
N	1.508961	0.470916	-0.601985
H	1.342854	-1.620454	-0.718391
H	1.636836	-0.823450	-2.270189

H	2.975628	-1.033057	-1.101114
H	1.680510	0.455295	0.417526
H	2.071591	1.227239	-0.992627
O	-1.034903	0.803268	-1.096730
H	-1.236372	1.747902	-1.172292
H	0.003277	0.732884	-0.869666
O	-2.388124	-0.251304	0.966249
H	-2.769564	-1.089814	0.670648
H	-1.908971	0.125484	0.171043
O	-0.754901	-0.380078	3.095019
H	-1.154191	0.208840	3.750903
H	-1.375128	-0.354469	2.310925
O	1.730699	0.367622	2.319095
H	0.825002	0.096700	2.636770
H	2.342941	-0.229291	2.771335
O	-0.575337	-0.208881	-3.689553
H	-1.359858	-0.612122	-4.086149
H	-0.874085	0.122412	-2.811867

(CH₃NH₂)(H₂O)₅- D 0.92 kcal/mol

C	-1.073144	0.567499	2.860112
N	-0.429808	-0.517944	2.103108
H	-1.112506	1.465191	2.232906
H	-2.104228	0.292492	3.111305
H	-0.547877	0.826384	3.791817
H	0.541475	-0.252097	1.861816
H	-0.362856	-1.355664	2.682137
O	-1.599947	-0.957350	-0.241205
H	-1.174898	-0.827801	0.699939
H	-2.229382	-1.688920	-0.172948
O	2.538677	0.236124	-1.329462
H	1.675594	-0.071828	-1.744688
H	3.218492	-0.349268	-1.691754
O	0.227059	-0.613095	-2.338664
H	-0.288148	-0.981099	-1.584191
H	-0.358782	0.123852	-2.613802
O	2.298049	0.207291	1.347687
H	2.721876	1.021932	1.651165
H	2.415518	0.211414	0.354110
O	-2.070419	1.053059	-2.111366
H	-2.059628	0.449596	-1.330313
H	-2.034477	1.948191	-1.745848

(CH₃NH₂)(H₂O)₅- E 1.65 kcal/mol

C	-1.527003	1.269908	-0.000138
N	-1.071907	-0.130849	0.000157
H	-1.138556	1.777284	0.889306
H	-1.140902	1.776114	-0.891263
H	-2.621712	1.363784	0.001275
H	-1.405770	-0.603948	0.846928
H	-1.407027	-0.604690	-0.845677
O	1.515355	0.173598	-2.690580

H	1.797135	1.065352	-2.938156
H	1.628385	0.115891	-1.701710
O	-1.132228	-0.566168	2.927061
H	-0.180472	-0.290412	2.949249
H	-1.221812	-1.226616	3.627491
O	-1.131817	-0.568008	-2.926842
H	-0.180253	-0.291593	-2.949009
H	-1.220671	-1.229307	-3.626565
O	1.515938	0.171629	2.690348
H	1.628419	0.114730	1.701345
H	1.800285	1.062298	2.938882
O	1.502234	-0.249339	-0.000152
H	1.767533	-1.182587	-0.000249
H	0.404929	-0.243499	-0.000804

(CH₃NH₂)(H₂O)₅- F 1.81 kcal/mol

C	-1.441580	1.348098	0.093141
N	-1.067683	-0.074286	0.020241
H	-0.980958	1.800062	0.978430
H	-1.067093	1.865911	-0.796153
H	-2.528359	1.502503	0.146673
H	-1.408799	-0.571686	0.850328
H	-1.436442	-0.491878	-0.841706
O	1.506641	0.050014	-2.700360
H	1.842186	0.921483	-2.953304
H	1.623942	-0.009488	-1.711439
O	-0.983146	-0.929517	2.880468
H	-0.135226	-0.418027	2.907793
H	-1.492468	-0.618109	3.641339
O	-1.194994	-0.461619	-2.905897
H	-0.222073	-0.271961	-2.936629
H	-1.345127	-1.130647	-3.587623
O	1.361976	0.512954	2.583968
H	1.568373	0.251002	1.644042
H	2.157767	0.307911	3.094410
O	1.491325	-0.319671	-0.006934
H	1.702190	-1.264458	0.054412
H	0.390928	-0.258492	-0.001053

(CH₃NH₂)(H₂O)₅- G 2.99 kcal/mol

C	-0.943872	-0.410531	-2.737697
N	0.476603	-0.157081	-2.441394
H	-1.477010	-0.598881	-1.799150
H	-1.379296	0.483750	-3.198249
H	-1.114412	-1.262771	-3.413976
H	0.896620	-0.968516	-1.983981
H	1.003629	-0.003439	-3.300914
O	2.191575	-0.894841	0.649501
H	3.012875	-1.117053	1.109651
H	1.461716	-1.024495	1.320975
O	-0.781003	1.554434	1.366699
H	-0.023160	1.613114	0.675705

H	-1.033147	2.461813	1.584969
O	-2.168052	-0.686621	0.649336
H	-3.061884	-0.749385	1.014674
H	-1.860932	0.234456	0.853125
O	1.174417	1.498491	-0.327630
H	1.737205	0.798665	0.083235
H	0.863006	1.034800	-1.163509
O	0.089523	-0.980209	2.351289
H	-0.689304	-1.256214	1.819207
H	-0.060570	-0.013133	2.400614

(CH₃NH₂)(H₂O)₅- H 3.65 kcal/mol

C	1.306398	1.531242	-1.973393
N	0.872780	0.227861	-1.454792
H	0.478041	2.004680	-2.512709
H	1.579834	2.181494	-1.134684
H	2.169967	1.471955	-2.653053
H	0.598246	-0.395310	-2.216309
H	1.616864	-0.225516	-0.911584
O	-1.850723	-0.998454	-2.542669
H	-1.916215	-0.719873	-1.602572
H	-2.574545	-1.626279	-2.672895
O	-1.355899	1.471982	2.478858
H	-0.797085	0.687847	2.669967
H	-0.813421	2.235822	2.721589
O	2.470778	-0.852313	0.862168
H	3.054590	-1.603384	1.035808
H	1.669099	-1.009156	1.415930
O	-0.012153	-1.027994	2.151276
H	-0.546770	-0.833402	1.310037
H	-0.379373	-1.839974	2.529084
O	-1.268326	-0.090813	0.050978
H	-1.533631	0.707735	0.549983
H	-0.422862	0.161617	-0.509579

(H₂SO₄)(CH₃NH₂)- A 0.00 kcal/mol

C	0.440903	0.015631	-3.159459
N	-0.604904	-0.036693	-2.113962
H	1.409695	0.110888	-2.662748
H	0.426232	-0.904752	-3.749388
H	0.281610	0.877345	-3.813456
H	-0.548257	0.781475	-1.434264
H	-1.548584	-0.130997	-2.491517
S	0.143699	0.019674	0.936270
O	1.312992	0.059729	1.787792
O	-0.133350	1.231114	0.129010
O	0.040659	-1.209383	0.091394
H	-0.406003	-0.790245	-1.356219
O	-1.155651	-0.037956	1.932034
H	-0.842162	-0.443463	2.759916

(H₂SO₄)(CH₃NH₂)- B 0.14 kcal/mol

C	0.442062	0.018073	-3.155434
N	-0.606411	-0.037615	-2.112845
H	1.411533	0.083401	-2.655237
H	0.411130	-0.886884	-3.768225
H	0.300012	0.898684	-3.787765
H	-0.533251	0.766975	-1.409853
H	-1.551093	-0.106395	-2.493378
S	0.144164	0.015755	0.935294
O	1.312262	0.060089	1.788248
O	-0.123126	1.224237	0.116333
O	0.033602	-1.217980	0.102254
H	-0.424035	-0.807052	-1.377038
O	-1.157488	-0.019180	1.929295
H	-0.850412	-0.423273	2.760279

(H₂SO₄)(CH₃NH₂)- C 0.16 kcal/mol

C	0.440045	0.018779	-3.160079
N	-0.603900	-0.038606	-2.113079
H	1.411658	0.085656	-2.664248
H	0.407925	-0.886200	-3.772794
H	0.293826	0.899169	-3.791776
H	-0.530492	0.765828	-1.409872
H	-1.550100	-0.108406	-2.489752
S	0.143760	0.016011	0.935845
O	-0.130440	1.223714	0.118170
O	1.316651	0.062604	1.782082
O	-1.152594	-0.019588	1.936265
H	-0.844453	-0.433714	2.761905
O	0.031094	-1.218332	0.103871
H	-0.419186	-0.808118	-1.378049

(H₂SO₄)(CH₃NH₂)(H₂O)- A 0.00 kcal/mol

C	-1.157325	0.386100	3.099759
N	-0.423183	-0.472500	2.142273
H	-2.215267	0.110645	3.106883
H	-0.741790	0.283296	4.106318
H	-1.065144	1.424757	2.772031
H	-0.807837	-0.344337	1.116176
H	0.605444	-0.220886	2.079022
S	-0.172285	-0.116921	-1.293505
O	-1.274030	-0.095829	-0.281944
O	-0.601697	-0.540577	-2.607097
O	0.289094	1.459462	-1.434187
H	-0.248209	1.834917	-2.154042
O	1.041455	-0.745964	-0.747846
H	-0.491004	-1.462217	2.388739
O	2.182633	-0.002075	1.524679
H	2.616677	0.861372	1.470500
H	1.910288	-0.226050	0.587154

(H₂SO₄)(CH₃NH₂)(H₂O)- B 0.20 kcal/mol

C	-1.198731	-0.461467	2.676114
---	-----------	-----------	----------

N	-0.465603	0.698765	2.107812
H	-0.972284	-1.331041	2.054213
H	-0.879238	-0.646510	3.705248
H	-2.273602	-0.265349	2.645929
H	-0.741322	0.834197	1.054114
H	-0.650447	1.560015	2.625183
S	-0.206490	-0.102287	-1.197802
O	-1.044599	0.867243	-0.428480
O	-0.873215	-0.659032	-2.353325
O	1.057257	0.790425	-1.762290
H	0.771002	1.160465	-2.616238
O	0.474027	-1.048265	-0.294307
H	0.575489	0.507659	2.091413
O	2.067326	-0.206139	1.663105
H	1.655957	-0.578461	0.831692
H	2.823522	0.319208	1.364277

(H₂SO₄)(CH₃NH₂)(H₂O)- C 2.53 kcal/mol

C	0.548846	-0.042966	3.678472
N	-0.534607	-0.119298	2.674299
H	1.492997	0.097588	3.146285
H	0.382551	0.802484	4.351664
H	0.593304	-0.971284	4.254445
H	-0.340967	-0.850286	1.902143
H	-1.458396	-0.255916	3.086497
S	0.042739	0.076173	-0.404342
O	0.048139	-1.185079	0.389996
O	1.230874	0.238895	-1.244945
O	-1.219827	-0.024742	-1.381880
H	-0.877420	-0.148658	-2.322094
O	-0.249796	1.240592	0.470539
H	-0.536901	0.711958	1.998077
O	0.136043	-0.264343	-3.671346
H	0.100800	0.526579	-4.229666
H	0.845919	-0.080945	-3.007726

(H₂SO₄)(CH₃NH₂)(H₂O)- D 2.58 kcal/mol

C	-1.019458	-0.214799	3.234056
N	-0.463619	0.256491	1.947987
H	-2.111703	-0.198356	3.190672
H	-0.683403	-1.240290	3.407756
H	-0.676025	0.421282	4.054879
H	-0.743778	1.210454	1.699039
H	0.589882	0.228229	1.907058
S	-0.325756	0.053503	-1.257904
O	-0.257835	1.379773	-0.650843
O	-0.738533	-0.069489	-2.636188
O	1.320066	-0.373836	-1.248565
H	1.391731	-1.203674	-1.753183
O	-0.944655	-0.951639	-0.341800
H	-0.766710	-0.336038	1.087823
O	2.211308	-0.071638	1.345719

H	2.003569	-0.207735	0.384671
H	2.847803	0.658075	1.360919

(H₂SO₄)(CH₃NH₂)(H₂O)- E 4.53 kcal/mol

C	-0.829904	-0.416116	3.486862
N	-0.302246	0.611449	2.571609
H	-0.827866	-1.382771	2.972739
H	-0.176939	-0.498535	4.362392
H	-1.853384	-0.209558	3.829500
H	-0.879498	0.673254	1.725755
H	-0.310871	1.529541	3.015461
S	-0.274624	-0.092164	-1.367590
O	-1.134022	0.281162	-0.264901
O	0.372689	1.329100	-1.835875
O	0.950491	-0.900350	-0.874172
H	1.342887	-0.551347	0.076291
O	-0.809702	-0.744304	-2.531897
H	0.746362	1.191130	-2.725994
O	1.855220	-0.187059	1.326677
H	2.517407	0.515311	1.247407
H	1.053617	0.195761	1.896796

(H₂SO₄)(CH₃NH₂)(H₂O)- F 4.69 kcal/mol

C	-0.550427	-0.015357	2.945793
N	-1.441548	0.037371	1.755910
H	0.487954	-0.031775	2.590138
H	-0.720413	0.869154	3.565600
H	-0.766048	-0.918845	3.522245
H	-1.264121	-0.758344	1.075408
H	-2.433601	0.080374	1.995543
S	-0.060172	-0.007105	-1.064077
O	-0.671930	-1.206203	-0.455267
O	-0.655829	-0.025007	-2.577648
O	-0.557195	1.240796	-0.433597
H	-1.189225	0.825455	1.089087
O	1.395838	-0.052320	-1.209189
H	0.006943	0.412265	-3.141892
O	2.367851	-0.084617	1.465653
H	2.138684	-0.096763	0.508311
H	3.066085	0.581517	1.535044

(H₂SO₄)(CH₃NH₂)(H₂O)- G 4.73 kcal/mol

C	-0.548364	-0.025263	2.943430
N	-1.443080	0.012465	1.755511
H	0.489386	-0.005182	2.585615
H	-0.746153	0.843670	3.576892
H	-0.733104	-0.943989	3.506279
H	-1.226640	-0.763184	1.053472
H	-2.435599	0.006088	1.996880
S	-0.057949	0.007685	-1.063448
O	-0.626798	-1.209808	-0.429045
O	1.397693	-0.042148	-1.208313

O	-0.654234	0.056158	-2.575697
H	-0.056764	-0.479497	-3.128374
O	-0.597581	1.240929	-0.459476
H	-1.231025	0.822487	1.110946
O	2.366239	-0.055940	1.464318
H	3.041887	0.634262	1.522166
H	2.134392	-0.086828	0.507846

(H₂SO₄)(CH₃NH₂)(H₂O)- H 4.75 kcal/mol

C	-0.549462	-0.034936	-2.946446
N	-1.441333	0.020380	-1.757159
H	0.489082	-0.010988	-2.591490
H	-0.736219	-0.962146	-3.494538
H	-0.747849	0.824179	-3.593064
H	-1.233110	0.841299	-1.130246
H	-2.434393	0.006581	-1.996152
S	-0.058039	0.009519	1.064442
O	-0.596073	1.246925	0.470826
O	1.397341	-0.045926	1.209238
O	-0.655067	0.043553	2.576842
H	-0.060984	-0.501606	3.123881
O	-0.628469	-1.203318	0.419468
H	-1.219618	-0.744556	-1.039857
O	2.367801	-0.052458	-1.464579
H	3.038605	0.642968	-1.516423
H	2.134953	-0.091282	-0.508750

(H₂SO₄)(CH₃NH₂)(H₂O)₂- A 0.00 kcal/mol

C	-0.140230	1.184169	-3.260778
N	-0.011678	0.366856	-2.036310
H	-1.087319	1.729729	-3.237702
H	0.685713	1.898773	-3.314890
H	-0.117832	0.537922	-4.142744
H	-0.807834	-0.314835	-1.907000
H	0.887846	-0.176856	-1.984273
S	0.000771	0.149971	1.363120
O	1.166929	-0.721813	1.196947
O	-1.301536	-0.540312	1.321515
O	0.173468	0.673590	2.889934
H	-0.660042	1.113018	3.138357
O	0.029868	1.355717	0.504098
H	-0.017266	0.937726	-1.145819
O	-2.096719	-1.205795	-1.176104
H	-2.124302	-2.171551	-1.236531
H	-1.895161	-1.010952	-0.217476
O	2.160165	-1.143684	-1.276237
H	3.102087	-0.923947	-1.301079
H	1.887495	-1.033189	-0.323133

(H₂SO₄)(CH₃NH₂)(H₂O)₂- B 1.59 kcal/mol

C	-1.196143	-0.826130	2.817264
N	-1.326782	0.329195	1.894985

H	-0.308669	-1.393999	2.524613
H	-1.075239	-0.471292	3.844511
H	-2.080209	-1.465331	2.746346
H	-1.443572	-0.001845	0.881338
H	-2.113913	0.932278	2.141149
S	-0.140535	-0.015329	-1.335850
O	-1.358405	-0.509616	-0.640316
O	0.993431	-0.945307	-1.195556
O	-0.511390	-0.004809	-2.916308
H	-0.550175	-0.933406	-3.209131
O	0.156011	1.388217	-1.056413
H	-0.410280	0.913434	1.879783
O	2.127732	-0.898202	1.272419
H	3.077907	-1.074432	1.222214
H	1.789888	-0.994077	0.340269
O	1.012143	1.575934	1.610451
H	1.597731	0.773026	1.587362
H	0.873251	1.763587	0.652434

(H₂SO₄)(CH₃NH₂)(H₂O)₂- C 1.84 kcal/mol

C	0.221920	1.283318	-3.151904
N	0.039950	0.371729	-2.002858
H	-0.613465	1.987481	-3.195336
H	1.154307	1.841186	-3.030690
H	0.261881	0.710618	-4.082779
H	-0.848422	-0.187374	-2.044441
H	0.835064	-0.301250	-1.881130
S	-0.181667	0.252333	1.468983
O	-0.973358	-0.877671	0.969077
O	-0.398121	0.665893	2.836069
O	1.363325	-0.441143	1.462648
H	1.913746	0.120777	2.036656
O	-0.078989	1.365915	0.494878
H	-0.010156	0.883309	-1.067399
O	2.134173	-1.228457	-1.086523
H	1.945852	-1.002697	-0.141530
H	2.098738	-2.195539	-1.123720
O	-2.117339	-1.235718	-1.440605
H	-3.063748	-1.034776	-1.430881
H	-1.815834	-1.151639	-0.495394

(H₂SO₄)(CH₃NH₂)(H₂O)₂- D 4.79 kcal/mol

C	0.506210	1.164295	-2.527715
N	0.455757	-0.230110	-2.019029
H	0.905633	1.799025	-1.733191
H	1.151846	1.218657	-3.408230
H	-0.508199	1.480336	-2.781841
H	-0.140660	-0.275184	-1.128457
H	0.008936	-0.859198	-2.691267
S	-0.268626	0.209047	1.361819
O	-1.030598	-0.343260	0.198980
O	-1.051487	1.071888	2.219912

O	0.123129	-1.110721	2.256135
H	-0.550415	-1.172512	2.956288
O	1.046045	0.707373	0.926765
H	1.407278	-0.568237	-1.727300
O	2.785665	-0.617765	-0.641528
H	2.270999	-0.177766	0.088933
H	3.157179	-1.421893	-0.252079
O	-2.376728	-0.628430	-2.230507
H	-3.305327	-0.845228	-2.390443
H	-2.295030	-0.530446	-1.260088

(H₂SO₄)(CH₃NH₂)(H₂O)₂- E 6.89 kcal/mol

C	0.041783	-0.290310	-3.442537
N	-1.083591	-0.206592	-2.474771
H	0.977201	-0.157832	-2.883755
H	0.030504	-1.269695	-3.928205
H	-0.062435	0.496669	-4.194540
H	-1.059108	0.675085	-1.891757
H	-2.001109	-0.311869	-2.911143
S	-0.406272	0.155882	0.575551
O	-0.832877	1.280939	-0.278599
O	1.007640	0.239328	1.012328
O	-1.290951	0.272264	1.891745
H	-0.724225	-0.018462	2.675354
O	-0.718552	-1.155427	-0.051866
H	-0.980309	-0.890846	-1.658239
O	2.554572	0.087648	-1.369689
H	3.120949	0.872336	-1.369834
H	2.098765	0.120976	-0.497677
O	0.605508	-0.383110	3.643160
H	1.129931	-0.226800	2.821997
H	0.701909	-1.328797	3.830967

(H₂SO₄)(CH₃NH₂)(H₂O)₂- F 6.89 kcal/mol

C	0.041488	-0.292386	3.441900
N	-1.083923	-0.208632	2.474159
H	0.976803	-0.158359	2.883317
H	-0.063548	0.493559	4.194872
H	0.031137	-1.272389	3.926333
H	-0.979522	-0.891456	1.656376
H	-2.001318	-0.315902	2.910299
S	-0.406150	0.157324	-0.575668
O	-0.717133	-1.154829	0.050809
O	1.007698	0.242299	-1.012344
O	-1.290823	0.273770	-1.891879
H	-0.724851	-0.019836	-2.674923
O	-0.833980	1.281360	0.279056
H	-1.060595	0.673977	1.892751
O	2.554295	0.088906	1.369544
H	3.122777	0.872061	1.371317
H	2.098812	0.124878	0.497456
O	0.605606	-0.387353	-3.641495

H	1.129443	-0.228717	-2.820375
H	0.702484	-1.333483	-3.826788

(H₂SO₄)(CH₃NH₂)(H₂O)₂- G 7.66 kcal/mol

C	-1.951812	0.058024	-2.490879
N	-2.161434	0.102518	-1.019211
H	-0.876142	-0.044975	-2.689020
H	-2.493797	-0.796126	-2.906147
H	-2.326714	0.983529	-2.936280
H	-1.594365	0.850558	-0.524368
H	-3.144409	0.207748	-0.759447
S	-0.010926	-0.037132	1.327062
O	-0.469470	1.219389	0.702179
O	1.441395	-0.200319	1.414135
O	-0.522228	0.133989	2.865686
H	0.005425	-0.479511	3.408362
O	-0.712831	-1.222272	0.784554
H	-1.759041	-0.727468	-0.500623
O	2.868037	0.137696	-0.915670
H	3.218104	1.036346	-0.832719
H	2.378409	-0.015614	-0.069697
O	1.172322	-0.148079	-3.037439
H	1.785675	-0.033887	-2.262832
H	1.604773	-0.815507	-3.588026

(H₂SO₄)(CH₃NH₂)(H₂O)₂- H 7.70 kcal/mol

C	-1.951569	0.062597	-2.487765
N	-2.164546	0.104454	-1.016493
H	-0.875746	-0.043201	-2.683848
H	-2.494792	-0.789289	-2.906118
H	-2.323064	0.989978	-2.932098
H	-1.598888	0.852062	-0.519465
H	-3.148214	0.208483	-0.758990
S	-0.009396	-0.037772	1.325392
O	-0.469421	1.219481	0.703039
O	1.442903	-0.199724	1.411887
O	-0.521870	0.131787	2.863978
H	-0.011835	-0.499429	3.403256
O	-0.709807	-1.223228	0.781185
H	-1.762198	-0.726092	-0.499011
O	2.869406	0.146083	-0.917539
H	3.208792	1.049212	-0.838710
H	2.381739	-0.009178	-0.070861
O	1.170218	-0.157464	-3.032636
H	1.785576	-0.038389	-2.260177
H	1.598763	-0.832035	-3.577519

(H₂SO₄)(CH₃NH₂)(H₂O)₂- I 10.68 kcal/mol

C	-1.517794	-0.428322	3.137675
N	-1.500286	0.276496	1.838378
H	-0.596191	-1.010797	3.236649
H	-1.533500	0.308250	3.947657

H	-2.385785	-1.091386	3.246797
H	-1.543494	-0.381024	1.051349
H	-2.307192	0.894156	1.746267
S	0.019352	-0.257413	-1.780126
O	-0.843285	-0.898491	-0.812563
O	-0.849204	1.031850	-2.265007
O	1.253283	0.381848	-1.085668
H	1.031731	0.757032	-0.108547
O	0.475470	-0.955227	-2.950554
H	-0.452422	1.348660	-3.097600
O	0.797116	1.212057	1.232517
H	0.894582	2.170068	1.335931
H	-0.220578	0.916809	1.536425
O	1.923285	-0.543012	3.201057
H	1.713250	0.091644	2.485025
H	2.645407	-1.082548	2.849106

(H₂SO₄)(CH₃NH₂)(H₂O)₃- A 0.00 kcal/mol

C	-1.499230	-1.216467	2.905824
N	-0.721175	-0.363048	1.981664
H	-2.511163	-1.348799	2.514040
H	-1.017743	-2.194194	2.995595
H	-1.551343	-0.746071	3.891781
H	-1.178802	0.571750	1.827972
H	0.270071	-0.212771	2.309820
S	-0.161214	-0.170606	-1.557149
O	1.288264	-0.157108	-1.809664
O	-0.753471	1.142142	-1.288334
O	-0.842277	-0.581329	-2.975442
H	-0.341587	-1.341144	-3.323819
O	-0.564452	-1.217585	-0.591957
H	-0.661740	-0.784153	1.011508
O	-1.988161	1.869993	0.995427
H	-1.794402	2.805670	1.147721
H	-1.613939	1.666587	0.094906
O	1.921785	0.134223	2.596232
H	2.498633	-0.478307	3.073800
H	2.354391	0.257553	1.694368
O	2.999006	0.419974	0.191780
H	2.376488	0.180070	-0.549879
H	3.308623	1.311163	-0.024361

(H₂SO₄)(CH₃NH₂)(H₂O)₃- B 0.02 kcal/mol

C	-1.289141	1.378095	-2.876034
N	-0.736464	0.366487	-1.947797
H	-2.196442	1.809957	-2.445574
H	-0.550200	2.168002	-3.033802
H	-1.528130	0.910532	-3.835210
H	-1.424079	-0.397436	-1.729552
H	0.156370	-0.063485	-2.311891
S	-0.078097	0.104277	1.564680
O	1.275714	-0.471372	1.611010

O	-1.133980	-0.920210	1.500851
O	-0.289116	0.884982	2.976924
H	-0.165576	0.230148	3.687828
O	-0.235310	1.199936	0.595225
H	-0.511777	0.782573	-1.002016
O	-2.479319	-1.423430	-0.780979
H	-2.572718	-2.381722	-0.874333
H	-2.055338	-1.284027	0.111262
O	1.723797	-0.618728	-2.715450
H	1.845327	-1.549470	-2.949965
H	2.266772	-0.478133	-1.879299
O	2.975656	-0.094573	-0.442958
H	2.363758	-0.202823	0.337216
H	3.812139	-0.499374	-0.175755

(H₂SO₄)(CH₃NH₂)(H₂O)₃- C 0.05 kcal/mol

C	-1.476196	-1.221232	2.913861
N	-0.710221	-0.363318	1.983873
H	-2.489291	-1.362264	2.528123
H	-0.986461	-2.194985	3.002440
H	-1.526375	-0.749594	3.899339
H	-1.173549	0.569296	1.835200
H	0.283173	-0.209063	2.303772
S	-0.166764	-0.172000	-1.552246
O	1.279395	-0.170145	-1.823646
O	-0.742387	1.144175	-1.265155
O	-0.870462	-0.565728	-2.964428
H	-0.386756	-1.332593	-3.321215
O	-0.567411	-1.222061	-0.589379
H	-0.656568	-0.783975	1.013133
O	-1.996316	1.866032	1.010352
H	-1.810065	2.802802	1.165499
H	-1.619141	1.667820	0.110155
O	1.936426	0.140171	2.573681
H	2.518954	-0.467276	3.050878
H	2.363268	0.261736	1.668584
O	2.998428	0.423183	0.163534
H	2.371830	0.181533	-0.574449
H	3.306561	1.314176	-0.055460

(H₂SO₄)(CH₃NH₂)(H₂O)₃- D 0.06 kcal/mol

C	-1.485935	-1.219934	2.907988
N	-0.714079	-0.363096	1.981824
H	-2.498563	-1.356071	2.519266
H	-1.000376	-2.195854	2.995748
H	-1.536826	-0.750200	3.894345
H	-1.173943	0.571302	1.832770
H	0.278732	-0.212362	2.305324
S	-0.164688	-0.172106	-1.553145
O	1.282407	-0.175654	-1.819750
O	-0.736376	1.146327	-1.267587
O	-0.865430	-0.562825	-2.967452

H	-0.385281	-1.333106	-3.321732
O	-0.572529	-1.221000	-0.591690
H	-0.658826	-0.782759	1.010595
O	-1.988506	1.871314	1.006744
H	-1.794690	2.806337	1.163250
H	-1.612771	1.671442	0.106129
O	1.931235	0.134730	2.580652
H	2.511742	-0.473599	3.059212
H	2.360332	0.256096	1.676829
O	2.997018	0.422073	0.171741
H	2.372958	0.180131	-0.568057
H	3.304138	1.313887	-0.045313

(H₂SO₄)(CH₃NH₂)(H₂O)₃- E 0.20 kcal/mol

C	0.059857	0.027107	-3.763071
N	0.010472	0.008634	-2.284602
H	0.752587	0.803865	-4.098787
H	0.401896	-0.943710	-4.132406
H	-0.936323	0.234517	-4.163760
H	-1.141785	1.765000	-0.113818
H	-0.630238	-0.747936	-1.916318
S	0.000698	-0.007272	1.587351
O	-0.024567	-1.401153	1.130244
O	-1.215211	0.764048	1.264302
O	0.007787	-0.182293	3.203325
H	0.027441	0.710873	3.592543
O	1.239555	0.715618	1.239993
H	0.965372	-0.161383	-1.859419
O	-1.023481	2.220344	-0.995251
H	-0.342878	0.922595	-1.885828
H	-0.435074	2.965916	-0.805573
O	-1.471274	-1.971458	-1.059772
H	-2.410962	-1.831057	-0.872188
H	-1.016538	-1.850014	-0.180149
O	2.425304	-0.259633	-0.973515
H	2.096392	0.098811	-0.101803
H	2.721599	-1.157978	-0.764069

(H₂SO₄)(CH₃NH₂)(H₂O)₃- F 0.44 kcal/mol

C	-0.002258	0.062076	3.831765
N	0.021135	0.003218	2.354313
H	0.467123	0.990131	4.169337
H	-1.036572	0.031417	4.185366
H	0.543458	-0.790106	4.246958
H	1.006134	0.018219	1.971860
H	-0.436601	-0.871918	1.980158
S	-0.004842	-0.002083	-1.656609
O	-1.140758	-0.847367	-1.275784
O	1.312684	-0.542598	-1.270710
O	-0.063243	-0.080674	-3.279681
H	0.641312	0.499712	-3.620558
O	-0.160165	1.423252	-1.313494

H	-0.847869	1.897782	0.139391
O	2.453757	0.080661	1.065905
H	3.186973	-0.540372	1.179133
H	2.090579	-0.105868	0.152493
O	-1.282688	-2.077945	1.100215
H	-0.923779	-2.968751	0.980449
H	-1.265881	-1.672432	0.187451
O	-1.219955	2.078340	1.050109
H	-0.498498	0.820873	1.922854
H	-2.180377	2.060314	0.927593

(H₂SO₄)(CH₃NH₂)(H₂O)₃- G 0.77 kcal/mol

C	-1.739759	-1.046888	-2.838653
N	-0.822023	-0.317231	-1.937381
H	-1.394189	-2.077383	-2.958742
H	-2.745055	-1.056299	-2.408608
H	-1.766244	-0.558042	-3.816565
H	0.168759	-0.303354	-2.304868
H	-1.143597	0.668656	-1.758685
S	-0.136854	-0.215679	1.573214
O	-0.754616	1.114354	1.441927
O	1.331304	-0.168427	1.658029
O	-0.638779	-0.816816	2.999121
H	-0.235843	-0.268627	3.696694
O	-0.661052	-1.216578	0.629312
H	-0.782912	-0.754671	-0.975351
O	2.809928	0.686027	-0.427324
H	3.738037	0.614820	-0.166046
H	2.281957	0.387223	0.363417
O	-1.500551	2.155587	-0.928966
H	-2.372399	2.565836	-0.843772
H	-1.251529	1.863192	-0.009081
O	1.831193	-0.265847	-2.700897
H	2.278868	0.071596	-1.865509
H	2.267112	-1.106542	-2.900340

(H₂SO₄)(CH₃NH₂)(H₂O)₃- H 0.88 kcal/mol

C	0.150005	-0.098695	-3.830704
N	0.047129	-0.002026	-2.358327
H	0.631513	-1.041946	-4.102305
H	-0.848464	-0.060995	-4.275548
H	0.746353	0.733018	-4.216700
H	1.000991	-0.032786	-1.896960
H	-0.419564	0.889573	-2.045911
S	0.006734	-0.005448	1.670120
O	-0.193528	1.357765	1.168020
O	1.344801	-0.561174	1.395192
O	-0.060419	0.216799	3.279273
H	0.094618	-0.650651	3.695393
O	-1.081443	-0.945217	1.347541
H	-0.527986	-0.795174	-1.954260
O	2.433178	-0.161088	-1.003877

H	3.012834	0.609534	-0.919095
H	2.085665	-0.320015	-0.077620
O	-1.260774	2.109909	-1.164377
H	-1.114849	3.063110	-1.242117
H	-0.954695	1.871374	-0.244420
O	-1.364843	-1.993359	-1.094354
H	-1.259254	-1.676221	-0.150912
H	-2.320607	-2.084379	-1.218314

(H₂SO₄)(CH₃NH₂)(H₂O)₃- I 1.64 kcal/mol

C	-1.069963	-1.260114	3.410214
N	-0.493611	-0.404335	2.352494
H	-2.006993	-1.697117	3.054971
H	-0.369523	-2.063205	3.655517
H	-1.266239	-0.664767	4.306381
H	-1.140766	0.368390	2.045640
H	0.426229	0.033813	2.613500
S	0.510425	-0.098274	-0.901967
O	1.565823	0.731225	-0.310530
O	-0.725428	0.675726	-1.233466
O	1.097824	-0.591617	-2.294322
H	0.343178	-0.625738	-2.962264
O	0.200829	-1.304413	-0.104220
H	-0.278913	-0.928165	1.454752
O	-2.046512	1.454499	1.014656
H	-1.923282	2.408987	1.120180
H	-1.623801	1.234936	0.138428
O	1.943056	0.875475	2.354901
H	2.809884	0.519314	2.595527
H	1.913492	0.847912	1.357882
O	-1.133338	-0.337220	-3.740894
H	-1.344160	0.174551	-2.923742
H	-1.048882	0.325089	-4.443036

(H₂SO₄)(CH₃NH₂)(H₂O)₃- J 1.68 kcal/mol

C	0.648836	-1.108231	-3.648667
N	0.316842	-0.310388	-2.449964
H	1.506860	-1.750527	-3.433179
H	-0.206460	-1.731555	-3.923751
H	0.895359	-0.443907	-4.481669
H	1.118599	0.283311	-2.110811
H	-0.515205	0.322019	-2.576805
S	-0.407949	-0.265957	0.887569
O	-1.327761	0.800753	0.464658
O	0.952590	0.262680	1.214465
O	-0.971945	-0.878619	2.241761
H	-0.460891	-0.476630	3.013199
O	-0.362753	-1.399603	-0.054691
H	0.063873	-0.901266	-1.607775
O	2.264894	1.050748	-1.036406
H	2.319822	2.017336	-1.028303
H	1.860341	0.807849	-0.157786

O	-1.801728	1.404707	-2.110929
H	-2.735313	1.257243	-2.317980
H	-1.719273	1.238525	-1.129591
O	0.726066	0.299178	3.928026
H	1.313372	-0.330234	4.372570
H	1.140298	0.466490	3.047463

(H₂SO₄)(CH₃NH₂)(H₂O)₃- K 1.85 kcal/mol

C	-1.110131	-1.254364	-3.362355
N	-0.537881	-0.374545	-2.321453
H	-0.395210	-2.045320	-3.604023
H	-2.035273	-1.703762	-2.991744
H	-1.326395	-0.674625	-4.264157
H	0.376266	0.064808	-2.600693
H	-1.190800	0.391975	-2.018464
S	0.538379	-0.053130	0.904378
O	-0.637807	0.803522	1.248895
O	1.622838	0.686549	0.253497
O	1.142895	-0.536389	2.292301
H	0.386594	-0.599336	2.955161
O	0.122541	-1.261559	0.155746
H	-0.314616	-0.886982	-1.418414
O	2.024749	0.601357	-2.411871
H	2.395232	1.448680	-2.695754
H	2.007377	0.638645	-1.415490
O	-1.102643	-0.309070	3.722486
H	-1.302844	0.223101	2.916503
H	-1.705360	-1.066749	3.683715
O	-2.094415	1.454276	-0.943694
H	-1.608188	1.281227	-0.088792
H	-2.100156	2.416930	-1.042464

(H₂SO₄)(CH₃NH₂)(H₂O)₃- L 2.24 kcal/mol

C	0.520644	-0.878971	-3.276961
N	0.540382	-0.223034	-1.951216
H	1.184759	-1.747583	-3.272956
H	-0.499146	-1.199054	-3.507367
H	0.857076	-0.169616	-4.037774
H	1.502784	0.082716	-1.650550
H	-0.123410	0.618949	-1.892826
S	0.083445	-0.065445	1.448544
O	-0.349336	1.303893	1.194221
O	1.536511	-0.270332	1.556268
O	-0.519301	-0.374330	2.925569
H	-0.095304	-1.191503	3.245424
O	-0.543532	-1.067494	0.537971
H	0.199548	-0.841580	-1.186028
O	2.931113	0.352088	-0.690524
H	3.315021	1.236988	-0.608251
H	2.534371	0.155964	0.201027
O	-1.275212	1.722795	-1.447921
H	-2.033829	1.096169	-1.346765

H	-0.987344	1.839683	-0.513772
O	-2.816493	-0.507064	-0.903073
H	-2.140031	-0.760771	-0.226607
H	-3.666152	-0.514645	-0.440072

(H₂SO₄)(CH₃NH₂)(H₂O)₃- M 2.54 kcal/mol

C	2.598585	-0.165907	-2.360453
N	1.380962	-0.190663	-1.523285
H	3.204495	0.700562	-2.083007
H	3.181812	-1.077812	-2.204368
H	2.321295	-0.085429	-3.415207
H	0.766872	0.695619	-1.623283
H	0.753172	-0.988357	-1.725524
S	0.026253	0.027094	1.617895
O	-0.931379	-1.024474	1.239229
O	-0.389244	1.394742	1.279579
O	0.000896	-0.071509	3.238354
H	0.451665	0.722395	3.578955
O	1.415599	-0.274294	1.205175
H	1.580731	-0.250861	-0.486438
O	-0.306903	1.883635	-1.487211
H	-1.144055	1.470492	-1.821495
H	-0.409847	1.891583	-0.505238
O	-0.989218	-1.815470	-1.269229
H	-1.247011	-2.746293	-1.329901
H	-0.986673	-1.588213	-0.286221
O	-2.405878	0.310483	-2.363627
H	-3.250337	0.458192	-1.913270
H	-2.051395	-0.530197	-1.983771

(H₂SO₄)(CH₃NH₂)(H₂O)₃- N 3.04 kcal/mol

C	-0.247883	-1.307404	2.548428
N	-0.667758	0.120453	2.517804
H	-0.021161	-1.614025	1.523493
H	0.650798	-1.411899	3.162171
H	-1.053858	-1.925016	2.953636
H	-1.531464	0.239702	1.906593
H	-0.887243	0.463823	3.455254
S	-0.125429	-0.079208	-1.411077
O	-1.553643	-0.446706	-1.397449
O	0.737221	-1.029626	-0.695973
O	0.361769	-0.268744	-2.953212
H	-0.200334	0.303815	-3.506247
O	0.107444	1.334555	-1.068942
H	0.848076	1.690148	0.504360
O	2.933883	-0.390144	0.766424
H	3.736312	-0.241281	0.246387
H	2.243334	-0.677481	0.113881
O	1.217351	1.614209	1.422024
H	1.998455	1.014878	1.281429
H	0.129000	0.748463	2.096600
O	-2.816628	0.257585	0.839032

H	-2.408180	-0.005853	-0.039407
H	-3.234439	1.114276	0.668650

(H₂SO₄)(CH₃NH₂)(H₂O)₄- A 0.00 kcal/mol

C	0.257010	1.970753	-2.844995
N	0.199979	0.753403	-2.004187
H	-0.713443	2.473217	-2.824495
H	1.022148	2.648828	-2.457236
H	0.500116	1.696867	-3.875446
H	-0.554937	0.093229	-2.336561
H	1.122308	0.241755	-1.999072
S	-0.124684	0.389855	1.619504
O	1.284635	0.372616	2.038628
O	-0.637370	-0.963383	1.326639
O	-0.963616	0.953302	2.897763
H	-0.639356	0.476354	3.683135
O	-0.460636	1.382663	0.589345
H	-0.031559	0.999643	-1.005955
O	-2.764525	-1.457122	-0.244578
H	-3.520596	-0.955049	0.091657
H	-2.015313	-1.254009	0.381971
O	2.526900	-0.726218	-1.877294
H	3.414187	-0.438467	-2.133331
H	2.612010	-1.048154	-0.924982
O	2.663221	-1.519199	0.648127
H	2.212782	-0.824209	1.199656
H	2.126487	-2.312897	0.793360
O	-1.939844	-0.838836	-2.685812
H	-2.305472	-1.090293	-1.781381
H	-1.846444	-1.673417	-3.166645

(H₂SO₄)(CH₃NH₂)(H₂O)₄- B 0.36 kcal/mol

C	-1.158136	0.559965	-3.662590
N	-0.673639	0.142638	-2.328133
H	-1.686772	-0.267995	-4.143324
H	-1.837373	1.410277	-3.555528
H	-0.309008	0.856413	-4.284290
H	0.020999	-0.642068	-2.398446
H	-0.152522	0.935996	-1.833433
S	-0.147580	-0.032367	1.872952
O	-0.252306	1.365163	1.424546
O	1.019860	-0.755902	1.346402
O	0.183976	0.013389	3.466089
H	-0.601104	0.378948	3.912609
O	-1.412893	-0.776883	1.756690
H	-2.221536	-0.784116	0.281783
O	2.681215	-0.060367	-0.549218
H	3.602848	-0.095368	-0.255964
H	2.116641	-0.284777	0.254318
O	0.780771	2.027190	-1.008023
H	1.647735	1.574208	-0.944849
H	0.414392	1.920330	-0.091377

O	-2.656605	-0.753815	-0.618751
H	-1.467419	-0.165901	-1.703855
H	-3.476737	-0.259347	-0.479074
O	1.477308	-1.647732	-2.402358
H	1.367341	-2.539460	-2.040575
H	2.037480	-1.165855	-1.735779

(H₂SO₄)(CH₃NH₂)(H₂O)₄- C 0.61 kcal/mol

C	-1.097975	0.487201	-3.710658
N	-0.645729	0.128243	-2.348293
H	-1.617529	-0.360514	-4.166136
H	-1.777986	1.341960	-3.657162
H	-0.234433	0.754912	-4.325551
H	0.042949	-0.664812	-2.365695
H	0.397930	1.930784	-0.131886
S	-0.155239	-0.037411	1.859835
O	-0.331528	1.332371	1.352542
O	1.109379	-0.676961	1.469394
O	0.026164	0.081294	3.473294
H	-0.825556	0.383958	3.836800
O	-1.342960	-0.886054	1.658956
H	-2.219534	-0.764341	0.232466
O	2.703004	-0.021680	-0.503837
H	3.631099	-0.031766	-0.229592
H	2.160675	-0.230483	0.318173
O	0.790402	2.037081	-1.036625
H	1.653551	1.580274	-0.948367
H	-0.128606	0.936499	-1.875757
O	-2.674476	-0.679826	-0.655062
H	-1.456084	-0.145137	-1.727277
H	-3.436455	-0.107204	-0.486765
O	1.473031	-1.700352	-2.266316
H	1.332939	-2.552550	-1.827461
H	2.044686	-1.180901	-1.639914

(H₂SO₄)(CH₃NH₂)(H₂O)₄- D 0.65 kcal/mol

C	-1.034957	-1.311358	3.511301
N	-0.423285	-0.440886	2.483862
H	-2.111675	-1.380325	3.335387
H	-0.596748	-2.311551	3.452848
H	-0.856170	-0.894727	4.506597
H	-0.851187	0.519782	2.472510
H	0.619566	-0.347331	2.604433
S	-0.494125	-0.113673	-1.065715
O	0.892588	-0.278939	-1.592457
O	-0.727699	1.249366	-0.562839
O	-1.458016	-0.348496	-2.310717
H	-0.919227	-0.260789	-3.158331
O	-0.869537	-1.159266	-0.097747
H	-0.590455	-0.809522	1.504153
O	-1.711590	1.905238	1.852833
H	-1.474430	2.825020	2.036530

H	-1.445483	1.745871	0.905289
O	2.311396	-0.050257	2.577462
H	2.965220	-0.709124	2.850023
H	2.552643	0.189353	1.629728
O	2.867004	0.575572	0.054882
H	2.148703	0.264761	-0.562103
H	2.925443	1.529928	-0.097441
O	0.358415	-0.184030	-4.260692
H	0.496275	-1.025327	-4.721085
H	0.915765	-0.236406	-3.447732

 $(\text{H}_2\text{SO}_4)(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_4$ - E 1.10 kcal/mol

C	-0.550967	-2.104883	-2.686655
N	-0.250208	-0.878077	-1.913474
H	-0.607774	-1.866049	-3.752298
H	0.235933	-2.845465	-2.519578
H	-1.507714	-2.516912	-2.355772
H	-1.012433	-0.159025	-2.033843
H	-0.179359	-1.100307	-0.882927
S	0.221824	-0.494641	1.707009
O	-0.060965	-1.556400	0.729106
O	0.323783	0.838927	1.036378
O	-1.187866	-0.386648	2.554252
H	-0.924906	-0.244297	3.480963
O	1.263091	-0.757515	2.677295
H	-2.330314	1.335989	-1.135566
O	-2.102628	1.915657	0.401166
H	-2.706596	1.529826	1.053632
H	-1.209446	1.577702	0.676426
O	2.102836	0.420084	-2.619943
H	2.919618	-0.060821	-2.815701
H	2.305452	0.956674	-1.795127
O	-2.346550	0.921075	-2.051868
H	0.663376	-0.446670	-2.211621
H	-2.369586	1.662788	-2.672928
O	2.504862	1.703841	-0.327568
H	1.764246	1.404035	0.262786
H	2.495077	2.670459	-0.286870

 $(\text{H}_2\text{SO}_4)(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_4$ - F 1.10 kcal/mol

C	1.261558	-1.190997	-3.086542
N	0.867387	-0.293493	-1.978095
H	2.190966	-1.709273	-2.834923
H	0.469055	-1.924945	-3.256271
H	1.407654	-0.603560	-3.996925
H	1.607818	0.408291	-1.740551
H	-0.067211	0.210904	-2.173858
S	0.192971	-0.251564	1.599003
O	-1.018515	0.542597	1.835452
O	1.418371	0.549093	1.479382
O	0.377447	-1.191682	2.911415
H	0.388106	-0.603829	3.688836

O	0.047341	-1.270225	0.533891
H	0.693785	-0.814164	-1.090277
O	2.785954	1.284369	-0.750508
H	2.922799	2.242021	-0.755813
H	2.370041	1.078198	0.126489
O	-1.585837	0.752059	-2.263823
H	-2.039440	-0.036706	-1.873054
H	-1.696820	1.446170	-1.563270
O	-1.868206	2.357048	-0.056471
H	-1.556196	1.767035	0.674123
H	-1.462007	3.217873	0.114480
O	-2.309940	-1.564071	-0.923382
H	-1.594864	-1.517611	-0.245354
H	-3.135195	-1.608471	-0.419411

(H₂SO₄)(CH₃NH₂)(H₂O)₄- G 1.12 kcal/mol

C	1.255056	-1.187721	-3.090983
N	0.863268	-0.291544	-1.980617
H	2.185234	-1.705967	-2.842156
H	0.462393	-1.921743	-3.259649
H	1.398807	-0.599237	-4.001065
H	1.604253	0.410042	-1.744159
H	-0.071973	0.212700	-2.173487
S	0.195316	-0.251981	1.597659
O	-1.019630	0.535781	1.837825
O	1.415830	0.555505	1.473995
O	0.388943	-1.191034	2.909557
H	0.398665	-0.603090	3.686922
O	0.051669	-1.271523	0.533132
H	0.692069	-0.813226	-1.092937
O	2.787307	1.282494	-0.756699
H	2.924620	2.240094	-0.761212
H	2.372597	1.075976	0.120743
O	-1.591327	0.753217	-2.257779
H	-2.042673	-0.036606	-1.866494
H	-1.701333	1.446546	-1.556313
O	-1.870022	2.356212	-0.048225
H	-1.557398	1.764332	0.680600
H	-1.461303	3.215782	0.123073
O	-2.309764	-1.565403	-0.918307
H	-1.592719	-1.519704	-0.242322
H	-3.133552	-1.609056	-0.411857

(H₂SO₄)(CH₃NH₂)(H₂O)₄- H 1.36 kcal/mol

C	-2.232608	0.105083	2.932040
N	-1.093138	0.032998	1.991255
H	-2.999819	0.771569	2.529087
H	-2.658741	-0.892263	3.071763
H	-1.888368	0.489759	3.895941
H	-0.674220	0.983675	1.800133
H	-0.318424	-0.598503	2.344016
S	-0.523138	-0.287692	-1.580888

O	0.482787	-1.353263	-1.576529
O	0.032642	1.078855	-1.476078
O	-1.164765	-0.260901	-3.073468
H	-1.469921	-1.164837	-3.272703
O	-1.648328	-0.527847	-0.658105
H	-1.382929	-0.308625	1.040761
O	-0.073392	2.419554	1.024136
H	0.903324	2.418330	1.000919
H	-0.287927	2.154208	0.101611
O	1.093540	-1.411227	2.747346
H	1.137715	-2.326400	3.057027
H	1.642358	-1.378648	1.893730
O	2.394737	-1.214406	0.477554
H	1.768651	-1.415801	-0.256362
H	2.619291	-0.270207	0.315545
O	2.413686	1.519566	-0.232170
H	1.665682	1.345530	-0.860750
H	3.113887	1.931159	-0.759022

(H₂SO₄)(CH₃NH₂)(H₂O)₄- I 1.38 kcal/mol

C	-0.533899	0.090085	3.897079
N	-0.405575	0.054362	2.424886
H	-1.113925	-0.771752	4.238476
H	0.459194	0.059863	4.354047
H	-1.040351	1.010004	4.202427
H	-1.340156	0.062079	1.936250
H	0.160734	0.865609	2.037997
S	-0.226826	0.053586	-1.681584
O	-0.531040	1.356322	-1.093560
O	-0.855782	-1.085764	-0.962170
O	-0.973729	0.136528	-3.121065
H	-0.794951	-0.697230	-3.593395
O	1.194652	-0.197922	-1.973030
H	3.755340	-0.194467	-0.075988
O	-2.697042	-0.158065	0.862994
H	-3.037822	0.677054	0.507503
H	-2.162835	-0.530809	0.113908
O	0.906459	-2.004325	1.141416
H	0.096854	-0.811598	2.074756
H	0.347814	-1.944200	0.335068
O	2.815921	-0.140291	0.150707
H	2.317994	-0.148702	-0.715987
H	1.738968	-1.555728	0.872052
O	1.116319	1.947035	1.130216
H	1.897507	1.408785	0.874000
H	0.581210	1.964521	0.303502

(H₂SO₄)(CH₃NH₂)(H₂O)₄- J 1.49 kcal/mol

C	-0.660342	0.056028	-3.807424
N	-0.482346	0.017495	-2.339513
H	-1.219597	-0.824213	-4.136111
H	-1.209596	0.959154	-4.087784

H	0.317645	0.066231	-4.296635
H	0.074767	-0.823493	-2.029786
H	0.066382	0.855135	-1.972595
S	-0.265044	-0.015585	1.702802
O	-0.279773	1.377117	1.234323
O	0.940868	-0.775029	1.319911
O	-0.109066	0.035662	3.321051
H	-0.898453	0.484021	3.675221
O	-1.519457	-0.737669	1.435776
H	-2.416177	-0.359637	0.036382
O	1.168139	-1.983363	-1.300059
H	2.012017	-1.490090	-1.233648
H	0.867807	-1.969081	-0.367672
O	0.991834	1.992365	-1.151356
H	1.839922	1.530889	-0.966989
H	0.537584	1.950345	-0.274636
O	-2.815165	-0.149430	-0.853594
H	-1.407527	-0.002853	-1.831177
H	-3.350525	0.643002	-0.702860
O	2.907341	0.082851	-0.302181
H	3.791333	0.169560	0.082288
H	2.295825	-0.138271	0.451331

(H₂SO₄)(CH₃NH₂)(H₂O)₄- K 1.66 kcal/mol

C	0.000619	0.028918	3.824863
N	-0.231677	0.000692	2.364268
H	-0.154303	-0.970838	4.239601
H	1.028356	0.344720	4.023451
H	-0.689569	0.730908	4.301898
H	-1.208505	-0.291716	2.119126
H	-0.084071	0.945422	1.922026
S	-0.345923	-0.036873	-1.614216
O	0.751073	0.917202	-1.287988
O	-1.616288	0.354663	-0.999428
O	-0.650967	0.164870	-3.199030
H	0.043227	-0.310933	-3.689718
O	0.051905	-1.437261	-1.447406
H	0.889407	-1.865065	0.211552
O	-2.647722	-0.783381	1.231139
H	-3.563493	-0.496186	1.350743
H	-2.376753	-0.449754	0.336034
O	0.192792	2.387006	0.967586
H	-0.596057	2.921985	0.794700
H	0.394910	1.966261	0.091446
O	1.394724	-1.715342	1.042382
H	0.433455	-0.686727	1.873924
H	2.164659	-1.180302	0.716167
O	3.116339	0.063650	-0.124077
H	2.359657	0.390988	-0.669336
H	3.777047	-0.248404	-0.758632

(H₂SO₄)(CH₃NH₂)(H₂O)₄- L 1.96 kcal/mol

C	-2.403664	-1.079278	2.372973
N	-1.222459	-0.345176	1.869235
H	-3.285356	-0.797633	1.791066
H	-2.236217	-2.155722	2.276887
H	-2.571830	-0.832528	3.425016
H	-1.365960	0.697369	1.896718
H	-0.344855	-0.585943	2.408751
S	0.412202	0.345433	-1.198227
O	1.744129	-0.261434	-1.099038
O	0.298564	1.631832	-0.501649
O	0.151489	0.681159	-2.734938
H	-0.250090	-0.132190	-3.167677
O	-0.674227	-0.618219	-0.812593
H	-1.034029	-0.555428	0.851751
O	-1.538461	2.333114	1.324883
H	-1.205461	3.101930	1.809081
H	-0.901925	2.200751	0.569386
O	1.151946	-0.838818	3.155447
H	1.395899	-1.684850	3.556393
H	1.868238	-0.653947	2.466420
O	2.959653	-0.379430	1.291916
H	2.528926	-0.342036	0.391379
H	3.436428	0.459180	1.371975
O	-1.144288	-1.596063	-3.346195
H	-1.196097	-1.552413	-2.362318
H	-2.044139	-1.418707	-3.658340

(H₂SO₄)(CH₃NH₂)(H₂O)₄- M 2.03 kcal/mol

C	-1.024758	-1.372421	3.478992
N	-0.417231	-0.471847	2.475397
H	-2.099237	-1.450984	3.293773
H	-0.573509	-2.365497	3.401683
H	-0.858346	-0.975708	4.484514
H	-0.858026	0.483050	2.481599
H	0.623123	-0.367601	2.605153
S	-0.496903	-0.074918	-1.071624
O	0.893881	-0.198781	-1.599386
O	-0.767513	1.271957	-0.546994
O	-1.454405	-0.306266	-2.321986
H	-0.902277	-0.289773	-3.165806
O	-0.843440	-1.145741	-0.119285
H	-0.573400	-0.821048	1.486221
O	-1.739181	1.867228	1.889754
H	-1.505290	2.784717	2.088481
H	-1.480713	1.727584	0.937062
O	2.313151	-0.048582	2.586299
H	2.974515	-0.700511	2.857198
H	2.555047	0.200969	1.641514
O	2.870319	0.602806	0.070488
H	2.150193	0.310353	-0.553137
H	2.946712	1.557319	-0.072120
O	0.374003	-0.283629	-4.263328

H	0.925675	-0.274154	-3.444620
H	0.520624	-1.154513	-4.661762

(H₂SO₄)(CH₃NH₂)(H₂O)₄- N 2.04 kcal/mol

C	-2.521905	0.220851	2.509860
N	-1.221488	0.048548	1.825503
H	-3.214516	0.747957	1.848277
H	-2.940223	-0.756991	2.764401
H	-2.380223	0.804586	3.423387
H	-0.803605	0.982577	1.532210
H	-0.514612	-0.461812	2.417943
S	-0.415201	-0.306061	-1.610930
O	1.061740	-0.397348	-1.467688
O	-0.924799	1.059915	-1.671924
O	-0.752457	-0.880319	-3.091213
H	-0.465569	-1.811360	-3.117641
O	-1.109899	-1.194816	-0.658589
H	-1.310643	-0.492203	0.929937
O	-0.211706	2.350440	0.724042
H	0.761682	2.274833	0.600689
H	-0.549134	2.121993	-0.173066
O	0.865710	-1.207534	3.113767
H	0.879702	-2.097730	3.491966
H	1.497948	-1.230201	2.331616
O	2.417253	-1.113173	0.952334
H	1.875933	-1.184559	0.135987
H	2.772147	-0.205319	0.873778
O	2.379564	1.562104	-0.115881
H	2.979370	2.131266	-0.619410
H	1.933565	0.974862	-0.781664

(H₂SO₄)(CH₃NH₂)(H₂O)₄- O 2.17 kcal/mol

C	0.792926	-0.037869	-4.077921
N	0.372212	0.025959	-2.661201
H	1.633982	0.641131	-4.242799
H	1.098683	-1.058260	-4.324945
H	-0.038829	0.253102	-4.725909
H	0.059692	0.994001	-2.383849
H	-0.431205	-0.630828	-2.451453
S	-0.510661	-0.026696	1.198656
O	-0.702920	-1.390754	0.676545
O	-1.309677	0.978891	0.486015
O	-1.056809	-0.006776	2.694201
H	-0.273960	-0.078270	3.324522
O	0.939565	0.330658	1.290776
H	1.880266	-0.265381	-0.003112
O	-0.423996	2.434226	-1.575017
H	-1.137990	3.022994	-1.856883
H	-0.749815	2.003898	-0.735252
O	-1.558512	-1.742775	-1.824251
H	-2.504378	-1.541963	-1.870235
H	-1.325832	-1.655602	-0.853941

O	2.324743	-0.625456	-0.821916
H	1.160348	-0.248967	-2.007877
H	2.412917	-1.573562	-0.642051
O	1.290677	-0.023410	3.971682
H	1.453761	0.793250	4.466877
H	1.545336	0.180265	3.040067

(H₂SO₄)(CH₃NH₂)(H₂O)₄- P 2.27 kcal/mol

C	1.844507	1.435807	-0.017156
N	1.917651	-0.048493	0.001896
H	2.854654	1.851415	0.020311
H	1.345252	1.757182	-0.934397
H	1.266896	1.776916	0.844977
H	2.360806	-0.377956	0.893478
H	0.944231	-0.463560	-0.013513
S	-1.622325	-0.035321	-0.006098
O	-0.602423	-1.107171	-0.049557
O	-1.750480	0.669713	-1.292177
O	-3.047199	-0.774653	0.253214
H	-3.265489	-1.276145	-0.553277
O	-1.500439	0.839801	1.162557
H	-0.563854	0.348093	2.532606
O	0.046947	0.179470	-3.276217
H	-0.091946	0.911844	-3.892627
H	-0.624192	0.313379	-2.553187
O	2.545873	-0.564063	2.642732
H	1.629109	-0.310416	2.955380
H	2.711316	-1.440457	3.017969
O	0.046165	0.154637	3.294202
H	2.387698	-0.395637	-0.866248
H	-0.115731	0.859236	3.936822
O	2.547677	-0.583564	-2.638921
H	2.709672	-1.452892	-3.031381
H	1.629209	-0.324620	-2.936349

(H₂SO₄)(CH₃NH₂)(H₂O)₄- Q 2.66 kcal/mol

C	1.336006	-0.086198	3.509162
N	0.972153	-0.092954	2.075076
H	1.936640	0.801964	3.722394
H	0.427712	-0.058591	4.117689
H	1.913880	-0.981208	3.758022
H	1.822564	-0.100375	1.448589
H	0.378555	-0.908309	1.825445
S	-0.069470	0.016717	-1.848823
O	-1.103170	-0.939120	-1.387468
O	1.296765	-0.500298	-1.730625
O	-0.258503	0.110011	-3.460880
H	-1.102597	0.567893	-3.625419
O	-0.273772	1.376311	-1.332333
H	-0.611107	1.822909	0.372367
O	3.011838	0.038463	0.239938
H	3.754649	-0.570707	0.124922

H	2.438265	-0.092333	-0.566767
O	-1.123231	-1.795727	1.069867
H	-1.288340	-2.749366	1.071531
H	-1.092581	-1.518768	0.093814
O	-0.683775	1.880364	1.356999
H	0.368520	0.769070	1.815284
H	-1.541880	1.441768	1.578197
O	-2.761014	0.185312	2.104164
H	-2.336774	-0.623813	1.727107
H	-3.618188	0.257732	1.660198

(H₂SO₄)(CH₃NH₂)(H₂O)₄- R 3.40 kcal/mol

C	1.250582	1.600159	-1.519852
N	1.468309	0.136632	-1.368427
H	1.959090	1.998476	-2.250295
H	0.225681	1.776578	-1.855811
H	1.404394	2.081749	-0.551150
H	2.384908	-0.056577	-0.913994
H	0.764404	-0.276890	-0.704097
S	-0.373939	-0.124987	1.617872
O	-0.277410	-1.038949	0.446955
O	-1.526789	0.780074	1.531825
O	-0.648199	-1.074341	2.907663
H	-1.598742	-1.288102	2.913443
O	0.905982	0.506222	1.937733
H	0.443526	-1.807773	-4.081574
O	-1.791306	-1.035638	-1.997317
H	-2.103611	-0.115787	-1.805242
H	-1.441352	-1.309759	-1.125078
O	3.306056	-0.005184	0.694276
H	2.517485	0.109444	1.282131
H	3.838574	-0.700626	1.104325
O	0.340640	-0.979979	-3.592646
H	1.326110	-0.365076	-2.279835
H	-0.524940	-1.057460	-3.082517
O	-2.280618	1.500882	-1.022573
H	-3.150169	1.925231	-1.011779
H	-2.070845	1.304307	-0.073716

(H₂SO₄)(CH₃NH₂)(H₂O)₄- S 4.49 kcal/mol

C	1.276127	-0.085693	3.405967
N	0.884455	0.014732	1.979356
H	0.366401	-0.131414	4.010653
H	1.875720	-0.987660	3.554961
H	1.868515	0.789997	3.685221
H	0.288014	0.856361	1.808902
H	1.713822	0.061356	1.323994
S	-0.174405	-0.007135	-1.887366
O	1.155315	-0.642792	-1.872376
O	-0.195057	1.353101	-1.337700
O	-0.535092	0.256076	-3.448699
H	-0.524861	-0.608145	-3.898940

O	-1.237194	-0.890973	-1.372026
H	-1.064184	-1.609473	0.101774
O	-0.941855	1.999203	1.132485
H	-0.993672	2.961875	1.212313
H	-0.780953	1.810631	0.164056
O	2.878212	-0.029060	0.084125
H	3.360924	0.767883	-0.178415
H	2.299702	-0.247511	-0.701151
O	-0.919896	-1.933814	1.041329
H	0.296443	-0.806107	1.694120
H	-0.804683	-2.892266	0.976688
O	-2.066558	-0.031220	2.954063
H	-2.039327	0.723402	2.336982
H	-2.022333	-0.807914	2.365807

(H₂SO₄)(CH₃NH₂)(H₂O)₅- A 0.00 kcal/mol

C	1.260306	-2.007279	-2.735496
N	0.520747	-0.994418	-1.950310
H	2.241809	-2.177147	-2.284449
H	0.703128	-2.948246	-2.748269
H	1.392004	-1.648420	-3.759817
H	1.055037	-0.070005	-1.903016
H	-0.436806	-0.805449	-2.357770
S	-0.372627	-0.559724	1.646714
O	-1.809330	-0.347575	1.466819
O	0.390647	0.721215	1.681244
O	-0.181653	-1.219293	3.118809
H	-0.725193	-0.701822	3.740725
O	0.247830	-1.566203	0.782188
H	0.389656	-1.294648	-0.957566
O	3.008958	0.822058	0.808076
H	3.530064	0.035020	1.021252
H	2.133505	0.682030	1.245785
O	-1.954507	-0.272621	-2.888663
H	-2.690373	-0.858942	-3.113037
H	-2.272786	0.285309	-2.107042
O	-2.584411	1.172624	-0.773857
H	-2.460081	0.611472	0.025696
H	-1.886182	1.855865	-0.670810
O	1.886635	1.348097	-1.650173
H	2.440686	1.170116	-0.846293
H	1.211160	1.978578	-1.316443
O	-0.210833	2.629079	-0.173360
H	-0.026205	2.020426	0.591559
H	-0.191164	3.527000	0.188550

(H₂SO₄)(CH₃NH₂)(H₂O)₅- B 0.43 kcal/mol

C	-0.135835	-1.213974	-3.887221
N	-0.053139	-0.686034	-2.508778
H	-0.156032	-2.307060	-3.863949
H	-1.048352	-0.847994	-4.365844
H	0.731333	-0.881672	-4.464991

H	0.823202	-0.995923	-2.012290
H	-0.035954	0.376312	-2.471429
S	-0.005443	-0.293983	1.940746
O	-0.766507	0.967196	1.889358
O	1.352611	-0.176334	1.374073
O	0.325044	-0.558092	3.508906
H	-0.517154	-0.771836	3.950389
O	-0.752875	-1.465216	1.470520
H	-1.799091	-1.368247	-0.015484
O	2.205694	1.706440	-0.371931
H	2.717118	2.432929	0.012060
H	1.869597	1.174330	0.396407
O	-0.015747	2.019493	-2.040439
H	0.768915	2.072768	-1.443040
H	-0.794322	2.088687	-1.441079
O	-2.213438	-1.121878	-0.877345
H	-0.891454	-0.966657	-1.916557
H	-2.477567	-0.187241	-0.730607
O	2.290925	-1.195473	-1.073047
H	1.964455	-1.176552	-0.145448
H	2.731481	-0.327818	-1.140221
O	-2.180418	1.665117	-0.264272
H	-1.696411	1.453070	0.585363
H	-2.878004	2.292703	-0.027031

(H₂SO₄)(CH₃NH₂)(H₂O)₅- C 0.49 kcal/mol

C	-0.823293	0.065382	3.922780
N	-0.209440	0.022001	2.577630
H	-0.524015	-0.816381	4.496520
H	-0.497312	0.967480	4.447793
H	-1.912787	0.078677	3.828417
H	-0.520933	-0.829748	2.028537
H	-0.524085	0.844675	1.983662
S	0.105413	0.041553	-1.902169
O	0.448552	1.345296	-1.336956
O	-1.319512	-0.167789	-2.205770
O	0.871049	0.074203	-3.334709
H	0.691200	-0.772153	-3.783668
O	0.692176	-1.102561	-1.155898
H	2.242109	-0.530150	-0.438678
O	-2.990661	-0.091607	-0.133460
H	-3.923456	-0.104426	-0.391680
H	-2.466710	-0.109249	-0.984773
O	-1.229459	1.930619	0.880274
H	-2.016795	1.434027	0.566286
H	-0.631227	1.919016	0.097969
O	3.020187	-0.078615	-0.024446
H	0.843261	0.013620	2.631955
H	2.981734	0.812876	-0.406382
O	-1.109333	-1.982609	0.906317
H	-0.485841	-1.876916	0.152113
H	-1.930286	-1.551218	0.582766

O	2.552279	0.059187	2.581272
H	2.789763	0.002422	1.603693
H	3.122384	-0.582690	3.027096

(H₂SO₄)(CH₃NH₂)(H₂O)₅- D 0.56 kcal/mol

C	0.487297	0.617275	3.980003
N	0.318428	0.091087	2.605612
H	0.818576	-0.183104	4.647514
H	1.235907	1.413605	3.973131
H	-0.464977	1.016608	4.339066
H	-0.414487	-0.657813	2.575570
H	-0.418067	1.801894	0.050361
S	-0.151233	-0.099005	-2.022956
O	0.151426	1.247955	-1.504987
O	-1.236277	-0.794828	-1.316598
O	-0.807979	0.110297	-3.501676
H	-0.100313	0.432965	-4.088373
O	1.053300	-0.915588	-2.228402
H	3.085041	0.984256	-0.940123
O	-2.901628	0.086951	0.489287
H	-3.809841	0.149107	0.160865
H	-2.334492	-0.212030	-0.288290
O	-0.792530	1.949876	0.957721
H	-1.696809	1.579779	0.874993
H	-0.037777	0.855338	1.947173
O	3.169161	0.025906	-0.823387
H	2.419897	-0.343435	-1.366510
H	2.958152	-0.396485	0.735789
O	-1.952043	-1.552579	2.443463
H	-1.906016	-2.455688	2.097229
H	-2.422241	-1.031602	1.738223
O	2.804871	-0.646937	1.702813
H	3.214359	-1.516550	1.810738
H	1.233631	-0.282448	2.234741

(H₂SO₄)(CH₃NH₂)(H₂O)₅- E 0.69 kcal/mol

C	-1.225092	-0.213587	3.806534
N	-0.729250	-0.087404	2.418586
H	-1.353233	0.779851	4.245193
H	-2.184303	-0.739185	3.811968
H	-0.503522	-0.779132	4.402405
H	0.225892	0.381931	2.384878
H	-0.586893	-1.035254	1.957989
S	-0.317971	-0.143855	-1.884102
O	-0.798201	-1.449718	-1.451516
O	1.043924	0.185440	-1.369769
O	-0.150238	-0.332993	-3.490186
H	-0.124489	0.557683	-3.884259
O	-1.243476	0.985282	-1.715304
H	-2.022368	1.245192	-0.188361
O	2.369827	-1.310330	0.454987
H	3.169336	-1.726889	0.102911

H	1.942111	-0.838020	-0.311162
O	-0.160632	-2.420270	1.080827
H	0.808691	-2.306162	0.968416
H	-0.494224	-2.216326	0.175522
O	-2.444511	1.308161	0.709081
H	-1.399299	0.454070	1.815143
H	-3.350724	0.996495	0.572161
O	1.829970	0.878139	2.219526
H	1.811607	1.584782	1.521604
H	2.238404	0.117213	1.752622
O	1.528235	2.519015	0.059000
H	1.317467	1.794889	-0.579010
H	2.249207	3.022098	-0.344862

(H₂SO₄)(CH₃NH₂)(H₂O)₅- F 0.83 kcal/mol

C	0.390410	-0.917537	3.901934
N	0.285964	-0.353719	2.536657
H	-0.605086	-0.979138	4.349490
H	0.822556	-1.920667	3.850104
H	1.027894	-0.279049	4.519782
H	-0.176526	0.587060	2.557558
H	1.240863	-0.262511	2.096567
S	-0.147470	-0.137049	-1.999081
O	1.166857	0.210796	-2.551759
O	-0.747476	0.932408	-1.182538
O	-1.167298	-0.189448	-3.274970
H	-0.844671	-0.889969	-3.870651
O	-0.189288	-1.472292	-1.384554
H	-1.028922	-1.784161	0.105255
O	-2.725947	0.752665	0.513728
H	-3.573680	1.023545	0.133627
H	-2.044576	0.818832	-0.226912
O	2.848882	-0.039222	1.569369
H	3.467496	-0.781912	1.616525
H	2.955114	0.320846	0.633916
O	3.184959	0.851864	-0.896728
H	2.445767	0.599904	-1.516751
H	3.282224	1.809139	-0.998937
O	-1.350332	1.926339	2.539395
H	-1.951467	1.623498	1.806349
H	-1.028146	2.795785	2.260946
O	-1.454211	-1.777200	1.003145
H	-2.164292	-1.109920	0.900369
H	-0.338405	-0.964550	1.919153

(H₂SO₄)(CH₃NH₂)(H₂O)₅- G 1.03 kcal/mol

C	-0.634658	0.267735	4.128823
N	-0.258583	0.142424	2.702913
H	-1.707733	0.460736	4.212368
H	-0.392015	-0.658996	4.656433
H	-0.084734	1.096684	4.582890
H	-0.522676	1.008356	2.162707

H	0.786177	-0.016327	2.591610
S	-0.821939	-0.018013	-1.645465
O	0.166619	0.878335	-2.249620
O	-1.875612	0.636853	-0.867360
O	-1.676717	-0.668003	-2.866962
H	-1.040624	-1.069353	-3.486900
O	-0.198640	-1.167265	-0.935638
H	-1.066110	-1.752264	0.445783
O	-1.208641	2.248960	1.185156
H	-0.676431	2.990036	0.862026
H	-1.475811	1.745270	0.368801
O	2.420415	-0.160886	2.293025
H	2.977217	-0.755550	2.814963
H	2.515549	-0.479206	1.327664
O	2.926303	0.777399	-2.200028
H	1.947536	0.872871	-2.291195
H	3.253001	1.672480	-2.031045
O	2.537522	-1.016825	-0.159767
H	2.858270	-0.362796	-0.832250
H	1.610724	-1.181589	-0.441533
O	-1.469600	-1.946225	1.334800
H	-2.424011	-1.880996	1.181267
H	-0.762471	-0.663277	2.241687

(H₂SO₄)(CH₃NH₂)(H₂O)₅- H 1.05 kcal/mol

C	-0.635988	0.265138	4.130322
N	-0.259036	0.140685	2.704570
H	-1.708961	0.458985	4.213322
H	-0.394510	-0.662222	4.657376
H	-0.085656	1.093256	4.585431
H	-0.521648	1.007476	2.164905
H	0.785658	-0.018832	2.593848
S	-0.821614	-0.016912	-1.646279
O	0.168481	0.875703	-2.253400
O	-1.870465	0.641847	-0.864977
O	-1.682649	-0.663557	-2.865134
H	-1.050081	-1.067408	-3.487042
O	-0.200572	-1.168547	-0.938443
H	-1.069801	-1.750937	0.444061
O	-1.198976	2.252359	1.187085
H	-0.661275	2.990778	0.866930
H	-1.465689	1.750888	0.369263
O	2.419954	-0.162348	2.294556
H	2.977745	-0.756850	2.815639
H	2.513536	-0.480824	1.328988
O	2.928065	0.770799	-2.201768
H	1.949618	0.867100	-2.295329
H	3.255576	1.666324	-2.036721
O	2.534234	-1.018122	-0.158007
H	2.856859	-0.365694	-0.831173
H	1.607335	-1.181746	-0.440205
O	-1.475679	-1.943175	1.332298

H	-2.429379	-1.871061	1.177271
H	-0.763460	-0.663948	2.242297

(H₂SO₄)(CH₃NH₂)(H₂O)₅- I 1.12 kcal/mol

C	1.734379	1.698456	-0.302229
N	1.926619	0.237502	-0.103432
H	1.195893	1.867180	-1.239205
H	1.147124	2.097652	0.528095
H	2.710460	2.189222	-0.337417
H	2.424669	-0.190090	-0.925549
H	2.427641	0.041923	0.801033
S	-1.629508	-0.097842	0.447357
O	-2.402562	0.591263	-0.591185
O	-1.103400	0.759476	1.511014
O	-2.689006	-1.043593	1.244735
H	-3.221766	-1.514100	0.578063
O	-0.602380	-1.015389	-0.109756
H	0.997155	-0.241985	-0.048582
O	0.488189	-0.000977	3.585009
H	0.095116	-0.776859	4.009225
H	-0.146071	0.245232	2.862084
O	2.709614	-1.034955	-2.407059
H	3.232642	-0.762433	-3.173188
H	1.753810	-1.106255	-2.722329
O	-0.963818	1.394859	-2.786762
H	-1.548330	1.185444	-2.013398
H	-1.553180	1.761997	-3.460863
O	0.108274	-1.147588	-2.916792
H	-0.258545	-0.238165	-3.056068
H	-0.255254	-1.377893	-2.037170
O	2.915007	-0.071934	2.455037
H	3.447936	-0.810823	2.779664
H	2.050877	-0.107110	2.961359

(H₂SO₄)(CH₃NH₂)(H₂O)₅- J 1.12 kcal/mol

C	1.752935	1.748470	-0.846031
N	1.875160	0.287367	-0.608308
H	2.723075	2.147032	-1.154581
H	1.007345	1.928219	-1.625436
H	1.435023	2.239931	0.076965
H	2.549387	0.083002	0.174881
H	0.953494	-0.119599	-0.315083
S	-1.509857	-0.068060	0.871401
O	-1.835658	1.178412	0.179431
O	-1.157093	0.078876	2.288040
O	-2.921446	-0.875654	0.837046
H	-2.834269	-1.641251	1.433802
O	-0.541255	-0.918722	0.131408
H	2.144718	-0.217750	-1.491939
O	-0.587906	-1.206026	-2.766637
H	-0.915842	-0.272231	-2.824207
H	-0.731633	-1.412967	-1.820947

O	-1.371655	1.425473	-2.490587
H	-2.161765	1.755070	-2.942050
H	-1.621506	1.373146	-1.530425
O	2.056927	-1.183928	-2.915929
H	1.050676	-1.236193	-2.983190
H	2.382592	-0.992737	-3.805985
O	1.302478	-0.207227	3.403268
H	0.405561	-0.145130	2.979846
H	1.290672	0.453260	4.110498
O	3.347444	-0.084777	1.695255
H	2.608383	-0.137428	2.372213
H	3.893366	-0.869219	1.847192

(H₂SO₄)(CH₃NH₂)(H₂O)₅- K 1.17 kcal/mol

C	1.809289	1.713849	0.846767
N	1.846034	0.228729	0.859658
H	1.783734	2.061581	-0.188987
H	0.912823	2.057683	1.367522
H	2.704072	2.102089	1.339637
H	2.630933	-0.124264	0.251724
H	1.904421	-0.134668	1.844946
S	-1.601973	-0.052193	-0.242959
O	-1.993212	0.563859	-1.510855
O	-1.518873	0.855955	0.904094
O	-2.826908	-1.041470	0.179316
H	-3.107460	-1.518013	-0.623032
O	-0.402190	-0.922752	-0.358388
H	0.966946	-0.166958	0.446461
O	-1.002342	0.166323	3.478950
H	-1.721780	-0.376939	3.829715
H	-1.263755	0.377966	2.544742
O	3.513055	-0.452109	-1.197426
H	4.181856	-1.141154	-1.311540
H	2.753661	-0.690912	-1.823006
O	-0.320898	0.796212	-3.726980
H	-0.960620	0.770830	-2.975755
H	-0.138994	1.734816	-3.874899
O	1.364474	-1.059634	-2.592203
H	0.931558	-0.357953	-3.140165
H	0.699114	-1.205906	-1.886653
O	1.591110	-0.496107	3.515897
H	0.606627	-0.329597	3.593272
H	1.736727	-1.389938	3.855918

(H₂SO₄)(CH₃NH₂)(H₂O)₅- L 1.20 kcal/mol

C	-0.349698	-0.037396	4.307624
N	-0.143726	-0.063770	2.842318
H	-1.370501	0.285748	4.529570
H	-0.189707	-1.037422	4.720152
H	0.356903	0.659091	4.767277
H	-0.331808	0.881113	2.411894
H	0.846892	-0.341038	2.599403

S	-0.636802	0.082588	-1.370312
O	0.660539	0.749333	-1.691552
O	-1.565245	0.926070	-0.609532
O	-1.373781	-0.127632	-2.769113
H	-0.669712	-0.334937	-3.455949
O	-0.417520	-1.246667	-0.768429
H	-1.297332	-1.698284	0.581799
O	-0.867408	2.277183	1.578014
H	-0.282791	3.012570	1.346393
H	-1.131770	1.866140	0.706577
O	2.476805	-0.653415	2.212940
H	2.743379	-1.583360	2.175883
H	2.648272	-0.299483	1.287632
O	2.877750	0.273317	-0.242635
H	2.035188	0.417793	-0.757682
H	3.371989	1.101358	-0.321666
O	0.855083	-0.333690	-4.249349
H	1.289686	-1.199827	-4.234124
H	1.167666	0.122972	-3.434786
O	-1.702484	-1.873093	1.480605
H	-2.644732	-1.682762	1.362213
H	-0.798428	-0.751549	2.370830

(H₂SO₄)(CH₃NH₂)(H₂O)₅- M 1.37 kcal/mol

C	1.266006	1.823810	-0.954174
N	1.593591	0.374391	-0.996328
H	0.290427	1.989225	-1.418252
H	1.228983	2.150193	0.088064
H	2.035825	2.385905	-1.489306
H	1.665555	0.027406	-1.991303
H	2.462284	0.178265	-0.447483
S	-0.339465	-0.289660	1.902463
O	-1.503974	0.592841	2.033020
O	0.942694	0.295579	2.291511
O	-0.546945	-1.468967	3.001239
H	-1.484210	-1.733817	2.970843
O	-0.281383	-0.970593	0.579241
H	0.848337	-0.172819	-0.500917
O	3.379266	0.023076	1.094187
H	3.877921	-0.763597	1.355934
H	2.573778	0.033882	1.670954
O	1.524732	-0.565581	-3.575781
H	1.848158	-0.064927	-4.337766
H	0.538829	-0.710255	-3.741946
O	-2.188732	-0.575842	-1.486288
H	-1.618213	-0.905620	-0.759228
H	-2.397200	0.344580	-1.188247
O	-1.078673	-0.846341	-3.859803
H	-1.523688	-0.735355	-2.958861
H	-1.411570	-1.684223	-4.210770
O	-2.365782	1.879255	-0.243948
H	-3.207062	2.328098	-0.078573

H	-2.097511	1.496620	0.629770
(H ₂ SO ₄)(CH ₃ NH ₂)(H ₂ O) ₅ - N 1.49 kcal/mol			
C	1.700525	1.420992	-0.630741
N	1.846451	-0.040454	-0.396823
H	2.683657	1.855705	-0.828966
H	1.046376	1.583723	-1.491060
H	1.262780	1.884605	0.257035
H	2.521040	-0.221662	0.388115
H	0.922965	-0.451887	-0.096174
S	-1.516920	-0.059880	0.946469
O	-2.092890	0.761260	-0.118771
O	-1.020829	0.714173	2.096681
O	-2.807367	-0.902140	1.474579
H	-2.507677	-1.464054	2.212067
O	-0.544920	-1.069869	0.475700
H	2.131364	-0.523882	-1.284499
O	0.240889	0.500627	-3.776297
H	-0.682140	0.319588	-3.419378
H	0.133249	0.707621	-4.714609
O	-2.133576	-0.013496	-2.701696
H	-2.919877	0.424472	-3.056940
H	-2.130069	0.221094	-1.732690
O	2.240013	-1.066085	-2.952526
H	1.475148	-0.561171	-3.354842
H	2.050602	-2.000202	-3.120650
O	1.203123	0.173401	3.520871
H	0.371406	0.333161	2.994807
H	1.253970	0.914793	4.140734
O	3.317458	-0.243117	1.943478
H	2.561249	-0.091688	2.585429
H	3.753165	-1.052947	2.244174
(H ₂ SO ₄)(CH ₃ NH ₂)(H ₂ O) ₅ - O 1.70 kcal/mol			
C	0.391386	1.524967	2.545123
N	0.367169	0.043485	2.439067
H	1.231044	1.908553	1.961292
H	-0.543471	1.926266	2.147312
H	0.507688	1.815085	3.592476
H	1.289501	-0.367900	2.706928
H	-0.454767	-0.352246	2.943996
S	-1.224728	0.045473	-0.638308
O	-0.617124	1.359605	-0.945263
O	-2.411290	0.131264	0.210266
O	-1.724239	-0.598797	-1.991537
H	-0.940241	-0.654033	-2.641157
O	-0.195017	-0.891968	-0.075256
H	0.204896	-0.262384	1.438128
O	-2.284966	-0.575844	2.864446
H	-2.775241	-1.389940	3.044292
H	-2.440502	-0.382213	1.903098
O	3.021605	-0.657309	2.281229

H	3.586026	-1.393652	2.553744
H	2.970483	-0.704642	1.280499
O	1.701320	1.260261	-2.212715
H	0.841085	1.413554	-1.712364
H	1.933324	2.104265	-2.625866
O	2.549427	-0.772696	-0.358538
H	2.647544	0.014217	-0.930761
H	1.571293	-0.913272	-0.360672
O	0.364501	-0.684551	-3.608335
H	0.848347	-1.518027	-3.506004
H	0.966407	0.014882	-3.240600

(H₂SO₄)(CH₃NH₂)(H₂O)₅- P 1.98 kcal/mol

C	1.512747	-1.335533	-1.807505
N	1.608761	0.098849	-1.425555
H	2.393252	-1.618282	-2.390445
H	1.446473	-1.942370	-0.901859
H	0.608169	-1.479688	-2.404059
H	1.521151	0.704869	-2.273064
H	0.791142	0.384012	-0.804842
S	-1.295287	-0.224881	0.535988
O	-0.437721	-1.337339	1.030999
O	-2.258690	-0.651207	-0.477864
O	-2.182129	0.275816	1.753875
H	-1.554600	0.645440	2.457823
O	-0.453137	0.928767	0.118219
H	2.465247	0.279430	-0.862299
O	3.496632	0.149053	0.656116
H	2.857789	-0.072515	1.384510
H	4.052835	0.860687	1.002186
O	1.558503	-0.537089	2.490745
H	1.787864	-1.248706	3.107239
H	0.795624	-0.903125	1.918457
O	-0.365978	1.244747	3.467871
H	0.419211	0.692547	3.227983
H	-0.166592	2.124797	3.113300
O	-1.541716	-0.195983	-3.052048
H	-1.849920	-0.310945	-2.111090
H	-2.326070	-0.321571	-3.603015
O	0.570257	1.364887	-3.671092
H	-0.286960	0.885942	-3.495205
H	0.344001	2.305617	-3.652066

(H₂SO₄)(CH₃NH₂)(H₂O)₅- Q 2.06 kcal/mol

C	-0.588773	0.258783	3.918813
N	-0.166507	0.041989	2.516705
H	-0.334410	-0.615944	4.523926
H	-0.078391	1.137610	4.321579
H	-1.669526	0.421988	3.956229
H	-0.651556	-0.790102	2.087916
H	-0.452836	0.864805	1.900467
S	0.147746	-0.060227	-1.895817

O	0.106685	1.357019	-1.515689
O	-1.010673	-0.853642	-1.437276
O	-0.059966	-0.108536	-3.511027
H	0.633284	0.450030	-3.907250
O	1.437284	-0.711699	-1.621970
H	2.622253	0.009086	-0.640764
O	-3.116811	0.147998	-0.087232
H	-3.934436	0.300001	-0.582525
H	-2.436249	-0.131627	-0.757309
O	-1.154157	1.979458	0.867734
H	-2.005263	1.559838	0.612187
H	-0.633212	1.915100	0.030189
O	3.294616	0.361654	0.003933
H	0.875919	-0.114138	2.457072
H	4.158631	0.139648	-0.369537
O	-1.563574	-1.954743	1.142726
H	-1.136020	-1.894896	0.261346
H	-2.405042	-1.484585	0.973976
O	2.567457	-0.373379	2.438311
H	2.914205	-0.116361	1.529082
H	2.860005	-1.286481	2.570591

(H₂SO₄)(CH₃NH₂)(H₂O)₅- R 2.10 kcal/mol

C	-0.198603	-0.257753	-4.004471
N	-0.326723	-0.015803	-2.550132
H	0.858500	-0.259170	-4.284416
H	-0.633821	-1.231189	-4.244957
H	-0.723283	0.520530	-4.566383
H	0.088127	0.891412	-2.260189
H	-1.334235	-0.024355	-2.235657
S	-0.907224	-0.000035	1.530049
O	0.223463	-0.953226	1.563961
O	-2.132622	-0.609346	0.992786
O	-1.231387	0.373313	3.077980
H	-1.588589	-0.428979	3.500702
O	-0.573275	1.312432	0.968706
H	0.214923	-0.760963	-1.975143
O	-2.896679	-0.167881	-1.546922
H	-3.505146	0.584758	-1.534543
H	-2.684593	-0.340718	-0.588186
O	1.131812	-1.700613	-1.078765
H	0.740969	-1.686816	-0.178611
H	1.956083	-1.134772	-0.971341
O	2.861989	-0.204038	2.036345
H	1.908244	-0.457747	2.002487
H	3.303254	-0.931954	2.496869
O	3.121885	0.077503	-0.694075
H	3.196346	-0.003229	0.291350
H	2.580436	0.883958	-0.820774
O	0.999626	2.027208	-1.062136
H	1.114734	2.988128	-1.049205
H	0.463816	1.806001	-0.248094

$(\text{H}_2\text{SO}_4)(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_5$ - S 2.13 kcal/mol

C	-0.675990	-0.104760	-3.906975
N	-0.271252	0.144167	-2.505025
H	-1.731669	-0.388022	-3.940886
H	-0.520087	0.794514	-4.509786
H	-0.072398	-0.919475	-4.315144
H	-0.434856	-0.729044	-1.890639
H	0.751631	0.405704	-2.441684
S	0.102535	0.126016	1.854970
O	0.869074	-1.005618	1.268982
O	-1.192250	-0.291092	2.392021
O	0.986714	0.655540	3.112265
H	0.935473	-0.026909	3.806291
O	0.083291	1.310690	0.984883
H	-0.837169	0.896839	-2.064106
O	-2.983618	-0.788360	0.239644
H	-2.897750	0.111688	-0.134622
H	-2.556279	-0.693206	1.120003
O	2.434984	0.632248	-2.380677
H	2.769936	1.536761	-2.298567
H	2.747764	0.164654	-1.546326
O	3.145482	-0.574440	-0.131543
H	2.338147	-0.706412	0.436052
H	3.576188	-1.439704	-0.176299
O	-0.787997	-1.949042	-0.897505
H	-1.666906	-1.664510	-0.515594
H	-0.172520	-1.834068	-0.139958
O	-1.866842	1.735409	-0.759083
H	-1.187390	1.664914	-0.025555
H	-2.238664	2.626732	-0.697559

 $(\text{H}_2\text{SO}_4)(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_5$ - T 2.52 kcal/mol

C	-0.458936	0.681476	-4.148832
N	-0.268691	0.163027	-2.776110
H	-0.778029	-0.126766	-4.813027
H	-1.220101	1.466544	-4.141329
H	0.482703	1.099271	-4.514885
H	0.489363	-0.563299	-2.740407
H	0.039890	0.936616	-2.101706
S	-0.934608	-0.030087	1.657440
O	-0.933283	1.362590	1.189542
O	0.391800	-0.676670	1.655249
O	-1.256836	0.018272	3.252744
H	-2.135294	0.426911	3.357161
O	-1.993586	-0.854578	1.056170
H	-2.323779	-0.927747	-0.593502
O	2.324553	-0.128321	-0.161532
H	2.995792	-0.033312	0.550063
H	1.533040	-0.398432	0.375497
O	0.653211	1.990602	-0.990280
H	1.443075	1.480266	-0.698871

H	0.052056	1.920009	-0.207903
O	-2.492743	-0.959957	-1.577773
H	-1.155845	-0.250748	-2.383424
H	-3.394303	-0.626188	-1.686730
O	1.992254	-1.445580	-2.471299
H	2.002294	-2.405957	-2.352389
H	2.281910	-1.062889	-1.597080
O	3.063001	-0.077744	2.518944
H	3.192184	0.730216	3.036206
H	2.096274	-0.242077	2.544924

(H₂SO₄)(CH₃NH₂)₂- A 0.00 kcal/mol

C	-0.350623	0.066380	4.287988
N	0.368477	-0.607974	3.194394
H	-0.752700	1.012385	3.911619
H	-1.192508	-0.556135	4.608470
H	0.284255	0.276928	5.159420
H	1.135621	-0.027951	2.840922
H	0.759116	-1.500166	3.495645
S	0.042231	0.287485	0.001902
O	1.097819	0.895093	0.798049
O	-0.819162	1.155232	-0.786948
O	0.697673	-0.765402	-0.953522
H	0.199297	-0.729880	-1.921434
O	-0.864143	-0.570161	0.947587
H	-0.381744	-0.663440	1.919898
C	0.339578	-0.031325	-4.298809
N	-0.519537	-0.482451	-3.191618
H	0.982496	-0.857223	-4.620544
H	-0.227205	0.333067	-5.166429
H	0.982568	0.777194	-3.936716
H	-1.102853	0.281738	-2.837178
H	-1.135849	-1.241729	-3.479948

(H₂SO₄)(CH₃NH₂)₂- B 2.79 kcal/mol

C	0.322967	0.497860	4.093854
N	0.217289	-0.577164	3.086679
H	0.228927	1.455556	3.575252
H	-0.478245	0.408596	4.833231
H	1.293760	0.454292	4.595979
H	0.897434	-0.444267	2.248899
H	0.293858	-1.513855	3.483536
S	-0.177773	0.073065	0.053639
O	1.144079	-0.087218	0.740110
O	-0.289409	1.319567	-0.701028
O	-0.282531	-1.127283	-0.968690
H	-0.345567	-0.738300	-1.955419
O	-1.284076	-0.136174	1.036556
H	-0.660049	-0.485716	2.461155
C	0.826530	0.000236	-4.091622
N	-0.405187	0.035932	-3.290093
H	0.950301	-0.996255	-4.529641

H	0.845804	0.743560	-4.901833
H	1.679907	0.186352	-3.431106
H	-0.516293	0.940648	-2.820791
H	-1.231672	-0.130744	-3.862567

(H₂SO₄)(CH₃NH₂)₂- C 2.86 kcal/mol

C	0.222981	0.534735	4.093953
N	0.171160	-0.564931	3.109626
H	0.123160	1.477943	3.550437
H	-0.596906	0.444491	4.812526
H	1.179721	0.524846	4.624055
H	0.873226	-0.432247	2.286128
H	0.257219	-1.490618	3.529662
S	-0.122802	0.054877	0.059249
O	1.173558	-0.089601	0.796070
O	-0.230808	1.308126	-0.685007
O	-0.151271	-1.134009	-0.980804
H	-0.298938	-0.738340	-1.955444
O	-1.263361	-0.185670	0.994659
H	-0.687680	-0.506742	2.459725
C	0.718979	0.032892	-4.156854
N	-0.457982	0.046967	-3.276424
H	0.821568	-0.956356	-4.616221
H	0.679352	0.787542	-4.955717
H	1.612145	0.217130	-3.550673
H	-0.548628	0.945603	-2.791022
H	-1.318367	-0.122063	-3.795795

(H₂SO₄)(CH₃NH₂)₂- D 8.40 kcal/mol

C	2.055294	-0.138852	-2.114208
N	2.220865	0.229867	-0.683807
H	1.000399	-0.422605	-2.266053
H	2.307446	0.720031	-2.742779
H	2.715144	-0.977320	-2.354068
H	1.925183	-0.544918	-0.017038
H	3.162879	0.549605	-0.452393
S	-0.232293	-0.040118	1.286271
O	0.841353	-1.051415	1.168141
O	-1.579395	-0.508795	0.987859
O	-0.216156	0.305863	2.881992
H	-1.126862	0.561246	3.113859
O	0.133199	1.223014	0.592187
H	1.498545	0.939606	-0.357020
C	-1.869911	0.578771	-2.627877
N	-1.242729	-0.668556	-2.171428
H	-1.478661	1.410422	-2.030159
H	-1.608280	0.765648	-3.677591
H	-2.969419	0.598711	-2.543906
H	-1.464165	-0.812652	-1.181505
H	-1.636774	-1.463915	-2.673965

(H₂SO₄)(CH₃NH₂)₂(H₂O)- A 0.00 kcal/mol

C	-0.422698	0.831352	3.668611
N	-0.054468	-0.486926	3.095990
H	-0.255485	1.582889	2.892718
H	-1.480551	0.827642	3.944706
H	0.191946	1.055579	4.545184
H	0.956526	-0.490482	2.783966
H	-0.216792	-1.251524	3.753265
S	-0.593039	-0.014255	-0.221377
O	0.411574	0.902301	0.382530
O	-1.502745	0.644316	-1.152312
O	0.226669	-1.113735	-1.025967
H	0.171790	-0.878374	-2.057389
O	-1.294172	-0.788399	0.850787
H	-0.626337	-0.663656	2.161282
C	0.949598	0.607163	-3.962162
N	-0.076989	-0.338192	-3.497033
H	1.875835	0.064162	-4.180188
H	0.654712	1.170720	-4.859130
H	1.156779	1.320773	-3.157661
H	-0.932397	0.158499	-3.229353
H	-0.313271	-1.020634	-4.216039
O	2.349103	-0.133892	1.843806
H	2.799723	-0.859093	1.387127
H	1.741525	0.271586	1.151406

(H₂SO₄)(CH₃NH₂)₂(H₂O)- B 0.46 kcal/mol

C	0.068177	1.781466	-2.973223
N	-0.039696	0.303075	-2.964069
H	-0.894701	2.218809	-3.250612
H	0.322983	2.101776	-1.959434
H	0.839262	2.107548	-3.677654
H	-0.345414	-0.068567	-3.864977
H	0.879240	-0.158761	-2.693278
S	-0.737876	-0.522098	0.272570
O	0.392181	-1.466834	0.098491
O	-1.537188	-0.780262	1.462397
O	-0.080938	0.938414	0.425389
H	0.083472	1.096317	1.451620
O	-1.544546	-0.396758	-0.977686
H	-0.739110	-0.018040	-2.169473
C	1.329075	0.381201	3.572157
N	0.140530	1.065272	3.038343
H	2.210513	1.017402	3.434056
H	1.247704	0.124173	4.638268
H	1.483854	-0.542064	3.003568
H	-0.683702	0.460776	3.111815
H	-0.052971	1.929098	3.543424
O	2.026043	-1.100513	-1.926575
H	2.856086	-0.732248	-1.592783
H	1.465049	-1.289459	-1.105303

(H₂SO₄)(CH₃NH₂)₂(H₂O)- C 2.48 kcal/mol

C	0.634807	0.431241	-4.256051
N	-0.522823	0.465239	-3.343544
H	1.500894	0.080957	-3.687930
H	0.451742	-0.254286	-5.089350
H	0.843922	1.432442	-4.644930
H	-0.320707	1.007365	-2.400198
H	-1.382616	0.784750	-3.789007
S	-0.188995	-0.327997	-0.352231
O	-0.064061	1.068603	-0.918913
O	1.101074	-0.758851	0.250728
O	-1.265135	-0.316576	0.714434
H	-0.785139	-0.325680	2.008439
O	-0.601137	-1.269008	-1.442917
H	-0.674754	-0.466169	-2.815255
C	-1.033066	0.856178	3.812011
N	-0.398708	-0.270045	3.094361
H	-2.116801	0.711377	3.842363
H	-0.644527	0.946250	4.831596
H	-0.816920	1.775623	3.261701
H	0.644402	-0.136228	3.013730
H	-0.580284	-1.163801	3.553454
O	2.189135	0.280230	2.384808
H	2.991133	-0.226120	2.574631
H	1.874847	-0.044579	1.479855

(H₂SO₄)(CH₃NH₂)₂(H₂O)- D 3.28 kcal/mol

C	0.452953	0.618947	4.248103
N	0.174368	-0.539209	3.384510
H	0.642202	1.490361	3.612928
H	-0.426044	0.834361	4.864843
H	1.318973	0.472363	4.908756
H	0.963117	-0.730804	2.759367
H	-0.014371	-1.379462	3.929728
S	-0.465486	-0.042323	0.130442
O	0.927114	-0.212666	0.605487
O	-0.680752	1.249489	-0.573317
O	-0.913831	-1.183321	-0.718621
H	-1.014904	-0.654278	-2.248308
O	-1.384290	-0.023526	1.400155
H	-0.801297	-0.257028	2.275948
C	0.197188	0.081401	-3.860613
N	-0.973894	0.158261	-2.952121
H	0.108571	-0.801192	-4.500371
H	0.243380	0.981706	-4.480268
H	1.100586	0.006367	-3.241185
H	-0.876292	0.917993	-2.211254
H	-1.863980	0.251419	-3.443289
O	2.617297	-0.134387	-1.634708
H	2.070696	-0.201070	-0.814262
H	3.168666	0.646257	-1.483341

(H₂SO₄)(CH₃NH₂)₂(H₂O)- E 3.73 kcal/mol

C	1.362906	-0.111557	-3.926485
N	0.348715	-0.751304	-3.062849
H	1.648788	0.837320	-3.465511
H	2.245038	-0.752758	-4.008069
H	0.953053	0.079429	-4.922475
H	-0.473300	-0.108856	-2.841361
H	0.019757	-1.647927	-3.422655
S	-0.629971	0.401743	-0.331830
O	-1.207014	0.794258	-1.640319
O	-0.386323	1.508842	0.586554
O	-1.731327	-0.552946	0.287409
H	-1.491692	-0.802733	1.260654
O	0.602407	-0.444018	-0.529561
H	0.662402	-0.835276	-2.014095
C	2.217384	-0.176808	2.758513
N	0.926367	0.472843	3.035078
H	2.127952	-0.740500	1.824001
H	3.053174	0.531738	2.652589
H	2.459265	-0.880825	3.563386
H	0.987549	1.066586	3.861588
H	0.649378	1.066940	2.242304
O	-1.145121	-1.189506	2.732929
H	-0.356600	-0.566191	2.969817
H	-1.873521	-0.928460	3.315241

(H₂SO₄)(CH₃NH₂)₂(H₂O)₂- A 0.00 kcal/mol

C	1.720258	1.221778	2.841924
N	1.082417	-0.105039	3.009930
H	2.756678	1.092251	2.517052
H	1.172165	1.757529	2.061647
H	1.693675	1.790433	3.776638
H	1.602796	-0.701755	3.654326
H	0.087262	-0.005169	3.353744
S	-0.396632	-0.473736	0.000381
O	-1.612133	-0.462883	0.847428
O	-0.648199	-1.162416	-1.292625
O	0.043258	0.962217	-0.266773
H	0.259839	1.177208	-1.659499
O	0.746715	-1.168333	0.719325
H	0.976360	-0.617751	1.991107
C	-0.903409	1.330840	-3.464834
N	0.409654	1.251161	-2.780768
H	-1.420447	2.244541	-3.158629
H	-0.776886	1.320505	-4.551712
H	-1.489002	0.463706	-3.148372
H	0.906635	0.356395	-3.034417
H	1.005890	2.049229	-3.004457
O	1.248687	-1.348041	-3.093753
H	0.573341	-1.455725	-2.352583
H	2.072581	-1.708812	-2.736688
O	-1.594578	0.275150	3.361630
H	-2.201770	-0.313014	3.831987

H	-1.688606	0.026092	2.385242
(H ₂ SO ₄)(CH ₃ NH ₂) ₂ (H ₂ O) ₂ - B 1.61 kcal/mol			
C	-0.217191	-0.608682	-4.543378
N	0.171823	0.460535	-3.610351
H	-0.406716	-1.521266	-3.969098
H	-1.146638	-0.329528	-5.050908
H	0.547065	-0.824969	-5.303044
H	1.009987	0.201315	-3.082038
H	0.359283	1.336068	-4.097405
S	-0.329483	0.091568	-0.308938
O	0.912339	-0.426376	-0.924660
O	-1.059869	-0.930244	0.469669
O	-0.068765	1.310524	0.514769
H	0.120653	0.968613	1.990936
O	-1.277905	0.536081	-1.478077
H	-0.725570	0.567585	-2.399091
C	1.038947	-0.487952	3.257217
N	0.109845	0.654813	3.038149
H	2.022017	-0.242655	2.844269
H	1.097593	-0.723933	4.323455
H	0.639018	-1.344704	2.709403
H	-0.889755	0.358837	3.191626
H	0.342345	1.455773	3.627423
O	-2.351177	-0.485327	2.753635
H	-2.014926	-0.671124	1.827919
H	-3.195346	-0.027666	2.635109
O	3.154018	-0.114054	0.762209
H	3.753040	-0.823729	0.491350
H	2.388333	-0.196170	0.145141
(H ₂ SO ₄)(CH ₃ NH ₂) ₂ (H ₂ O) ₂ - C 1.75 kcal/mol			
C	0.302910	-0.489162	-4.579970
N	0.619667	-0.591499	-3.149096
H	-0.354227	0.373163	-4.740079
H	1.221089	-0.323150	-5.156027
H	-0.203395	-1.377839	-4.985941
H	-0.237767	-0.712539	-2.591072
H	1.207193	-1.404401	-2.964887
S	-1.033586	-0.107385	0.069958
O	-1.628459	-0.320324	-1.243921
O	-1.987944	-0.069666	1.187164
O	0.112875	-1.047234	0.320979
H	0.925661	-0.474505	1.461429
O	-0.363866	1.356957	0.114402
H	0.316185	1.444683	-0.649208
C	2.510217	-0.728782	2.908139
N	1.376655	0.025226	2.333581
H	3.299426	-0.838618	2.159311
H	2.909178	-0.215315	3.788012
H	2.157447	-1.721855	3.199195
H	0.562540	0.130640	3.007002

H	1.644624	0.961339	2.019944
O	-0.994958	0.319006	3.620333
H	-1.409222	-0.314513	4.223055
H	-1.466856	0.196687	2.739850
O	1.437185	1.535655	-1.772938
H	1.322056	2.333797	-2.308997
H	1.191749	0.737005	-2.389474

(H₂SO₄)(CH₃NH₂)₂(H₂O)₂- D 2.79 kcal/mol

C	-0.410761	-0.993800	-4.283596
N	-0.537958	0.218934	-3.447099
H	0.283008	-1.677875	-3.787975
H	-1.384004	-1.484745	-4.373644
H	-0.027158	-0.749418	-5.279411
H	0.395985	0.692230	-3.312740
H	-1.193152	0.890935	-3.849183
S	-0.391788	-0.000196	0.000005
O	0.444555	1.142432	-0.463288
O	0.444461	-1.142814	0.463470
O	-1.290019	0.465090	1.124704
H	-0.893094	0.058201	2.387481
O	-1.289788	-0.465472	-1.124876
H	-0.892892	-0.058112	-2.387523
C	-0.410602	0.994607	4.283107
N	-0.538130	-0.218469	3.447154
H	-1.383736	1.485789	4.373038
H	-0.026947	0.750583	5.278990
H	0.283255	1.678322	3.787112
H	0.395709	-0.692009	3.312926
H	-1.193427	-0.890155	3.849595
O	1.898837	-1.142738	2.627496
H	1.464682	-1.132715	1.712685
H	2.288956	-2.023188	2.717994
O	1.899178	1.142495	-2.627142
H	1.464939	1.132374	-1.712371
H	2.289484	2.022884	-2.717427

(H₂SO₄)(CH₃NH₂)₂(H₂O)₂- E 2.93 kcal/mol

C	0.571459	-0.169298	-4.302732
N	0.578986	-0.427504	-2.855300
H	0.130788	0.816439	-4.489903
H	1.598753	-0.156695	-4.685626
H	-0.002565	-0.910577	-4.877725
H	-0.379650	-0.436335	-2.478172
H	0.957158	-1.353362	-2.652969
S	-1.281531	-0.170540	0.087999
O	-1.973084	-0.227443	-1.193707
O	-2.125806	-0.260937	1.284285
O	-0.112462	-1.112667	0.122732
H	0.955908	-0.574980	1.080443
O	-0.616061	1.304075	0.246076
H	0.181416	1.375937	-0.368443

C	2.636050	-0.863049	2.398471
N	1.588787	-0.023875	1.779023
H	3.291864	-1.267150	1.622408
H	3.227287	-0.277098	3.108294
H	2.153500	-1.688429	2.928162
H	0.889002	0.338250	2.485660
H	1.972579	0.753017	1.230998
O	-0.572703	0.417014	3.409217
H	-0.874360	1.287325	3.707234
H	-1.226603	0.158107	2.695730
O	1.651513	1.290532	-1.150344
H	1.885665	2.108677	-1.612385
H	1.313109	0.624646	-1.888258

(H₂SO₄)(CH₃NH₂)₂(H₂O)₂- F 2.97 kcal/mol

C	0.573357	-0.167630	-4.299830
N	0.578483	-0.425247	-2.852253
H	0.135609	0.819224	-4.487947
H	1.601124	-0.158030	-4.681511
H	-0.002041	-0.907603	-4.875116
H	-0.380579	-0.431594	-2.476275
H	0.953806	-1.352084	-2.649063
S	-1.283826	-0.170540	0.087902
O	-1.977250	-0.225960	-1.192916
O	-2.126374	-0.261021	1.285470
O	-0.115379	-1.113437	0.120270
H	0.955495	-0.578365	1.078159
O	-0.617418	1.303799	0.246099
H	0.181331	1.374842	-0.366368
C	2.638258	-0.862924	2.393615
N	1.589512	-0.025696	1.773987
H	3.292488	-1.269059	1.617284
H	3.230886	-0.274751	3.100424
H	2.157049	-1.686855	2.926756
H	0.891022	0.337971	2.480977
H	1.971956	0.749620	1.222624
O	-0.569316	0.417594	3.407649
H	-1.224623	0.160449	2.694795
H	-0.870065	1.287317	3.708258
O	1.655109	1.287494	-1.144698
H	1.891393	2.105974	-1.605076
H	1.315739	0.623751	-1.884179

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- A 0.00 kcal/mol

C	2.069587	-0.526234	3.306038
N	0.872897	-0.041755	2.591206
H	1.970770	-1.597811	3.500911
H	2.957476	-0.353737	2.691199
H	2.183946	0.003231	4.256697
H	-0.021234	-0.210630	3.113717
H	0.925395	0.978647	2.340989
S	-0.857749	-0.103682	-0.322859

O	-1.792072	0.181864	0.788127
O	-1.469525	-0.682870	-1.521757
O	-0.166849	1.221985	-0.714920
H	0.473186	0.929672	-2.062394
O	0.254766	-1.031562	0.184039
H	0.723355	-0.529059	1.643749
C	-0.104063	0.588753	-4.094481
N	0.895744	0.531181	-3.000490
H	-0.349529	1.631670	-4.313393
H	0.286839	0.104993	-4.994885
H	-0.998726	0.071991	-3.737334
H	1.148735	-0.472166	-2.750459
H	1.752484	1.036190	-3.234396
O	1.479582	-1.955378	-1.991575
H	0.885348	-2.643684	-2.326925
H	1.053721	-1.686186	-1.116485
O	-1.709599	-0.689611	3.294379
H	-2.384070	-0.203953	3.789148
H	-1.864068	-0.449562	2.333161
O	0.908836	2.461843	1.385258
H	0.285075	3.144910	1.670592
H	0.480554	2.053142	0.569083

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- B 1.80 kcal/mol

C	1.049199	1.915770	2.627678
N	0.996491	0.460016	2.911006
H	2.017449	2.168152	2.186158
H	0.259856	2.136124	1.903823
H	0.895293	2.491092	3.545276
H	1.757200	0.160595	3.523013
H	0.066318	0.188606	3.348482
S	-0.523782	-0.650784	0.114190
O	-1.491035	-1.173391	1.106343
O	-0.626742	-1.346500	-1.186666
O	-0.721983	0.841643	-0.063456
H	-0.633497	1.221598	-1.528029
O	0.901797	-0.840442	0.670158
H	1.028797	-0.115625	1.957602
C	-1.818176	1.000423	-3.281723
N	-0.547124	1.368135	-2.613341
H	-2.620479	1.664904	-2.948804
H	-1.709912	1.062199	-4.368598
H	-2.056368	-0.025718	-2.989520
H	0.242456	0.695329	-2.902059
H	-0.272164	2.330812	-2.814292
O	1.223788	-0.598051	-3.055299
H	0.617045	-1.110475	-2.459499
H	2.005048	-0.457555	-2.461280
O	-1.546150	-0.222462	3.541693
H	-1.816694	-0.947912	4.121917
H	-1.630026	-0.588637	2.599858
O	2.995465	-0.305645	-0.946903

H	3.584838	-1.071663	-0.890666
H	2.232526	-0.524725	-0.336758

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- C 2.22 kcal/mol

C	0.110321	-0.949311	3.702461
N	-0.392380	0.368160	3.246977
H	-0.710578	-1.516985	4.149431
H	0.468622	-1.483534	2.818340
H	0.917547	-0.830118	4.432130
H	-0.826079	0.897159	4.005149
H	0.370799	0.951621	2.818256
S	-1.072390	-0.149003	0.026786
O	-0.320151	1.136772	-0.276352
O	-1.889906	-0.554336	-1.126238
O	-0.041914	-1.204202	0.380051
H	1.097280	-1.190001	-0.626638
O	-1.937574	0.064691	1.242124
H	-1.137231	0.233093	2.390820
C	3.158040	-0.633437	-0.657679
N	1.916508	-1.054383	-1.347543
H	3.515614	-1.435424	-0.004892
H	3.932687	-0.380438	-1.387712
H	2.928868	0.244995	-0.047089
H	1.563043	-0.280015	-2.020332
H	2.048246	-1.919247	-1.874568
O	0.910538	0.987461	-2.738912
H	0.155740	0.675346	-3.305754
H	0.436558	1.263892	-1.912178
O	1.394898	1.739331	1.615362
H	1.500463	2.701321	1.636970
H	0.751081	1.557222	0.848746
O	-1.462456	0.086515	-3.710422
H	-1.706309	-0.146450	-2.772015
H	-1.654656	-0.708186	-4.226880

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- D 2.90 kcal/mol

C	0.335056	-0.468114	3.945587
N	-0.622869	0.384571	3.197402
H	-0.190516	-1.343759	4.337602
H	1.115133	-0.801477	3.250196
H	0.777184	0.095884	4.772656
H	-1.426057	0.648800	3.771062
H	-0.171558	1.270322	2.830566
S	-0.932597	-0.293668	-0.274944
O	-0.490883	1.138602	-0.254206
O	-1.885820	-0.525549	-1.382630
O	0.313816	-1.160330	-0.494466
H	1.030070	-0.671581	-1.705026
O	-1.542344	-0.694959	1.032259
H	-1.003731	-0.116124	2.286765
C	2.092839	1.066226	-2.367457
N	1.437992	-0.236644	-2.642874

H	2.962306	0.908847	-1.723164
H	2.400485	1.545775	-3.301381
H	1.367247	1.690401	-1.839557
H	0.580453	-0.122232	-3.259074
H	2.077947	-0.902644	-3.078659
O	2.148091	-1.652207	1.461758
H	1.448221	-1.474640	0.779256
H	2.185278	-2.617770	1.513965
O	0.480150	2.439602	1.790153
H	0.088037	3.323563	1.754556
H	0.141879	1.964998	0.960125
O	-1.006671	0.112217	-3.779288
H	-1.433808	-0.092494	-2.883826
H	-1.430966	-0.490374	-4.406081

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- E 3.02 kcal/mol

C	0.302469	0.423889	4.868362
N	0.777030	-0.336575	3.701676
H	-0.346146	1.233835	4.519137
H	-0.294531	-0.231625	5.511158
H	1.114700	0.858566	5.467919
H	1.308079	0.257482	3.058837
H	1.374071	-1.115272	3.977572
S	-0.579320	-0.100062	0.613720
O	0.591096	0.755337	0.961618
O	-1.722841	0.667270	0.088735
O	-0.174030	-1.184250	-0.323361
H	-0.175439	-0.529066	-1.779350
O	-1.060451	-0.782965	1.941848
H	-0.311371	-0.680620	2.699625
C	-0.099066	1.348195	-2.781445
N	-0.253577	-0.130309	-2.776227
H	0.903352	1.593042	-2.423507
H	-0.236826	1.729787	-3.796688
H	-0.842906	1.778568	-2.107811
H	-1.211596	-0.389901	-3.068862
H	0.516768	-0.574154	-3.309228
O	-2.974735	-0.144808	-2.222916
H	-2.640458	0.096154	-1.318344
H	-3.634667	-0.835110	-2.070462
O	2.698585	0.373249	-0.732255
H	3.207090	1.189978	-0.633270
H	1.926887	0.464431	-0.105065
O	2.429005	-0.757597	-3.206614
H	2.585130	-0.390477	-2.294813
H	2.849342	-1.628825	-3.202458

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- F 3.99 kcal/mol

C	0.130475	-0.900322	4.547154
N	0.405987	-0.655933	3.118225
H	-0.370863	-0.021654	4.962322
H	-0.530641	-1.764911	4.654847

H	1.058362	-1.079076	5.099633
H	1.010437	0.196648	2.946697
H	0.852273	-1.451320	2.655408
S	-0.884515	0.119735	0.234526
O	-0.074560	1.386604	0.203303
O	-1.894883	0.117682	-0.850374
O	0.067233	-1.060107	0.075390
H	0.358049	-1.353727	-1.342547
O	-1.553449	-0.026775	1.570773
H	-0.509019	-0.435902	2.515838
C	1.968750	-1.348971	-2.780931
N	0.546722	-1.580558	-2.418426
H	2.610384	-1.954743	-2.134836
H	2.142346	-1.615289	-3.828133
H	2.167555	-0.282357	-2.626806
H	-0.095425	-0.948090	-2.956986
H	0.259268	-2.546145	-2.589635
O	-1.221598	0.354502	-3.352218
H	-1.564289	0.358222	-2.398054
H	-2.002548	0.361238	-3.922722
O	1.191098	1.724191	-2.312418
H	0.408827	1.665845	-2.888172
H	0.800460	1.695801	-1.408322
O	1.687029	1.554802	2.175305
H	1.052048	1.557104	1.388137
H	1.633739	2.446587	2.546889

(H₂SO₄)(CH₃NH₂)₂(H₂O)₃- G 4.45 kcal/mol

C	2.061581	0.494067	2.973580
N	1.106967	-0.600859	2.662480
H	3.022297	0.283068	2.495418
H	1.629801	1.417440	2.571881
H	2.199270	0.582925	4.055507
H	1.411194	-1.497521	3.046935
H	0.146117	-0.392913	3.032444
S	-0.665662	-0.682480	-0.350076
O	-1.553236	-1.116774	0.756286
O	-0.872936	-1.398700	-1.609613
O	-0.839036	0.819698	-0.573958
H	-0.185849	1.124421	-1.886747
O	0.798310	-0.888238	0.100850
H	0.984984	-0.723390	1.565332
C	-0.532129	0.772675	-3.968115
N	0.356550	1.179530	-2.852255
H	-1.355077	1.486832	-4.059404
H	0.026591	0.730710	-4.908166
H	-0.934337	-0.211978	-3.714831
H	1.158179	0.497405	-2.722792
H	0.737611	2.118243	-2.983116
O	-0.285297	2.328843	1.732021
H	-0.482466	1.868865	0.881766
H	-0.946965	1.949848	2.336386

O	-1.567018	0.023285	3.093474
H	-2.272594	-0.333403	3.650664
H	-1.693462	-0.387212	2.174692
O	2.290517	-0.638610	-2.103850
H	1.796566	-0.791091	-1.239546
H	2.216962	-1.489759	-2.561239

(H₂SO₄)(CH₃NH₂)₂(H₂O)₄- A 0.00 kcal/mol

C	2.082769	0.630512	3.659016
N	0.956252	0.096794	2.866514
H	2.877035	-0.117455	3.738633
H	2.476417	1.517277	3.154957
H	1.742411	0.910474	4.660153
H	0.545428	-0.746330	3.276089
H	0.150541	0.807922	2.739673
S	-0.163106	-0.734304	-0.100335
O	-0.818497	-1.461686	1.014503
O	-0.235512	-1.455914	-1.387016
O	-0.818776	0.638883	-0.258273
H	-0.849866	1.066617	-1.753113
O	1.293105	-0.497937	0.291839
H	1.228301	-0.165637	1.855457
C	-2.053108	0.617472	-3.434920
N	-0.841696	1.220049	-2.828907
H	-2.949172	1.123414	-3.064647
H	-2.007847	0.690008	-4.525335
H	-2.081079	-0.433215	-3.134507
H	0.047182	0.701870	-3.167373
H	-0.761979	2.216936	-3.036179
O	1.232531	-0.348950	-3.420635
H	0.817093	-0.982233	-2.780763
H	2.015087	-0.026399	-2.899050
O	-2.534025	-0.557206	2.845880
H	-3.460551	-0.766640	2.664691
H	-2.013099	-0.956515	2.092939
O	3.053991	0.437244	-1.530036
H	3.827242	-0.142860	-1.479451
H	2.431311	0.098278	-0.824904
O	-1.113484	1.704639	2.269902
H	-1.830305	1.089473	2.568447
H	-1.048992	1.485495	1.302513

(H₂SO₄)(CH₃NH₂)₂(H₂O)₄- B 2.87 kcal/mol

C	1.107472	1.687421	3.089271
N	0.694633	0.280273	3.319695
H	2.175493	1.723108	2.856809
H	0.541766	2.057180	2.229736
H	0.896535	2.296954	3.972589
H	1.240573	-0.163910	4.059773
H	-0.340344	0.221397	3.561183
S	-0.464755	-0.530728	0.257549
O	-1.692945	-0.828877	1.031178

O	-0.464332	-1.244374	-1.049507
O	-0.321376	0.955815	0.060015
H	0.153026	1.401767	-1.372124
O	0.758901	-1.003196	1.056529
H	0.790541	-0.300556	2.381882
C	-0.484820	1.867864	-3.364936
N	0.568127	1.594973	-2.352320
H	-0.988170	2.809266	-3.125310
H	-0.033465	1.934692	-4.359245
H	-1.216407	1.051409	-3.336893
H	1.124710	0.696594	-2.568003
H	1.230080	2.369636	-2.276464
O	1.774142	-0.791400	-2.604717
H	0.978332	-1.184570	-2.166596
H	2.440891	-0.844117	-1.872487
O	-2.002366	0.184780	3.425779
H	-2.545768	-0.432451	3.935543
H	-1.986619	-0.185543	2.482944
O	3.156114	-0.950966	-0.209780
H	3.546919	-1.830143	-0.101233
H	2.280506	-0.999873	0.269301
O	-2.486290	-0.687442	-2.862941
H	-3.348348	-0.694580	-2.423747
H	-1.854188	-0.967761	-2.158517

(H₂SO₄)(CH₃NH₂)₂(H₂O)₄- C 11.29 kcal/mol

C	-2.157230	-0.582396	3.073040
N	-1.043190	-1.267600	2.379804
H	-1.886247	-0.358349	4.109395
H	-2.358622	0.359498	2.554699
H	-3.051639	-1.212555	3.058308
H	-0.721222	-2.090794	2.891590
H	-1.291525	-1.566826	1.315113
S	1.737172	0.003300	0.509769
O	3.119422	-0.117396	0.898311
O	1.488891	0.790411	-0.726320
O	1.243603	-1.490041	0.215784
H	0.245737	-1.532180	-0.039709
O	0.838262	0.501227	1.618576
H	-0.217589	-0.614045	2.240431
C	-1.846056	-0.359722	-3.293136
N	-2.168607	0.018067	-1.891960
H	-2.378915	-1.277813	-3.560122
H	-2.142956	0.445074	-3.972056
H	-0.764180	-0.522841	-3.369831
H	-1.657110	0.927248	-1.605074
H	-3.171563	0.174645	-1.773284
O	-0.812047	2.204364	-1.157015
H	0.090721	1.802333	-1.064985
H	-1.018914	2.455802	-0.222859
O	1.405526	-0.474381	-3.219314
H	2.085702	-1.160373	-3.272085

H	1.559593	-0.049724	-2.343592
O	-1.002754	2.447476	1.589837
H	-0.675543	3.274555	1.972161
H	-0.227488	1.819409	1.616585
O	-1.329880	-1.748833	-0.122298
H	-1.463027	-2.672229	-0.382321
H	-1.855855	-0.756814	-1.183495

(H₂SO₄)₂(CH₃NH₂)- A 0.00 kcal/mol

C	3.693952	-0.322021	-0.689011
N	2.400406	0.406765	-0.678427
H	4.323760	0.030487	0.131422
H	3.488306	-1.386599	-0.556511
H	4.199544	-0.163754	-1.644844
H	2.520762	1.415420	-0.798848
H	1.742460	0.068207	-1.442549
S	-0.265904	-0.013452	2.165359
O	-0.357464	0.054192	3.588247
O	-0.867553	1.312538	1.565489
O	1.055282	-0.236294	1.562634
H	1.875081	0.246428	0.227063
O	-1.234223	-1.148839	1.671191
H	-1.285392	-1.161800	0.657241
S	-0.733094	-0.046261	-1.756571
O	-1.431521	-1.067189	-0.959441
O	0.511366	-0.488705	-2.398200
O	-1.684066	0.264126	-3.020704
H	-2.600903	0.332971	-2.695178
O	-0.549993	1.229105	-1.019693
H	-0.780836	1.307344	0.548458

(H₂SO₄)₂(CH₃NH₂)- B 3.15 kcal/mol

C	3.653736	0.374839	-0.721435
N	2.387026	-0.399138	-0.704286
H	4.139438	0.264662	-1.694178
H	3.415332	1.427200	-0.551099
H	4.317216	0.020407	0.071244
H	2.541068	-1.398003	-0.861867
H	1.882948	-0.292581	0.215403
S	-0.764078	-0.088751	-1.950754
O	-1.772951	-0.318073	-2.954683
O	-0.525539	-1.190019	-0.988249
O	0.514777	0.484425	-2.408348
H	1.697344	-0.057117	-1.447431
O	-1.399241	1.143360	-0.986946
H	-2.323794	1.251552	-1.275034
S	-0.244617	-0.014058	2.202992
O	-0.388719	-0.090747	3.620263
O	1.104953	0.079252	1.638959
O	-0.985504	-1.235358	1.552514
H	-0.839586	-1.245549	0.539614
O	-1.070454	1.248182	1.715168

H	-1.141012	1.251132	0.716728
(H ₂ SO ₄) ₂ (CH ₃ NH ₂)- C 3.17 kcal/mol			
C	3.195474	0.504155	1.041900
N	2.375179	-0.695091	0.723307
H	3.676772	0.369667	2.013681
H	3.949921	0.652623	0.265381
H	2.523978	1.364577	1.080726
H	1.588717	-0.820015	1.437175
H	1.896001	-0.589443	-0.209369
S	-0.157216	0.017902	-2.228903
O	-0.250055	0.190676	-3.642043
O	-1.324822	-0.964101	-1.797428
O	1.097320	-0.488195	-1.666411
H	2.939428	-1.547644	0.697751
O	-0.518704	1.375385	-1.527707
H	-0.386686	1.301512	-0.515937
S	-0.736461	0.096284	1.921105
O	-1.646152	0.608257	2.915417
O	0.269120	-0.879657	2.376661
O	-1.707073	-0.826275	0.892650
H	-2.626146	-0.625634	1.146847
O	-0.123801	1.092943	1.010812
H	-1.428908	-0.964191	-0.801638
(H ₂ SO ₄) ₂ (CH ₃ NH ₂)- D 3.57 kcal/mol			
C	3.007171	0.563056	-0.338762
N	2.276413	-0.732376	-0.369595
H	2.263475	1.363132	-0.340757
H	3.618314	0.624251	0.565224
H	3.636699	0.646234	-1.227976
H	1.640464	-0.780360	-1.240263
H	2.916776	-1.529476	-0.383697
S	-0.505245	0.105785	-2.235435
O	-0.923783	0.976853	-3.307223
O	0.687796	-0.728604	-2.485436
O	-0.368533	0.795989	-0.909878
H	1.658168	-0.821053	0.473680
O	-1.680835	-1.001105	-2.013099
H	-2.503770	-0.607956	-2.356252
S	-0.419415	-0.114845	2.347833
O	-1.123674	-0.505730	3.533834
O	0.703442	-0.917304	1.882285
O	-1.441003	0.132312	1.219437
H	-0.985479	0.379249	0.277453
O	0.266515	1.336473	2.583310
H	-0.387394	1.908172	3.028118
(H ₂ SO ₄) ₂ (CH ₃ NH ₂)- E 5.11 kcal/mol			
C	3.685922	0.010966	0.767633
N	2.210579	-0.050354	0.673452
H	4.053790	0.845353	0.165368

H	3.978628	0.154792	1.810699
H	4.112331	-0.922689	0.392542
H	1.854390	-0.193945	-0.301679
H	1.764336	-0.803352	1.243346
S	-0.275461	-0.094330	-2.317222
O	-0.232660	1.493125	-2.002392
O	-0.506037	-0.311880	-3.715390
O	0.968304	-0.562658	-1.723530
H	1.714199	0.789497	1.042833
O	-1.509515	-0.599019	-1.539283
H	-1.517432	-0.404764	-0.491568
S	-0.699868	0.005371	1.910338
O	0.065057	1.248338	1.794348
O	0.133287	-1.202858	2.029022
O	-1.494290	0.190728	3.306021
H	-2.115043	-0.556000	3.394890
O	-1.776435	-0.144377	0.895158
H	-1.011206	1.909948	-2.417890

(H₂SO₄)₂(CH₃NH₂)- F 8.89 kcal/mol

C	3.572370	0.013718	-0.575944
N	2.102121	-0.124104	-0.486899
H	3.839170	0.393156	-1.565425
H	3.923111	0.709807	0.190392
H	4.039240	-0.962402	-0.422108
H	1.669008	-0.739466	-1.228588
H	1.768127	-0.476152	0.433458
S	-0.601130	0.082922	-2.205451
O	-1.430209	0.316389	-3.361201
O	0.355610	-1.038705	-2.324289
O	-0.042878	1.249690	-1.511558
H	1.576084	0.757710	-0.666945
O	-1.699167	-0.465320	-0.999515
H	-2.154789	-1.249172	-1.354119
S	-0.330581	-0.095910	2.341227
O	0.703577	-0.962112	1.805250
O	-0.652431	-0.120327	3.735931
O	0.194976	1.375593	1.919249
H	-0.445941	2.042462	2.231383
O	-1.666411	-0.249268	1.554014
H	-1.560236	-0.329248	0.530435

(H₂SO₄)₂(CH₃NH₂)- G 8.99 kcal/mol

C	3.567823	0.025804	-0.574774
N	2.100372	-0.141079	-0.490323
H	3.831267	0.397322	-1.568156
H	3.899395	0.740172	0.183177
H	4.054989	-0.937664	-0.404789
H	1.685144	-0.773655	-1.223480
H	1.768672	-0.485662	0.433523
S	-0.599787	0.081408	-2.207298
O	-1.429086	0.329906	-3.359755

O	0.341695	-1.051220	-2.329363
O	-0.024984	1.241842	-1.513580
H	1.554649	0.727924	-0.688384
O	-1.701932	-0.452469	-0.998617
H	-2.163957	-1.233640	-1.350957
S	-0.330435	-0.095832	2.342722
O	-0.651593	-0.121344	3.737594
O	0.698573	-0.966340	1.803988
O	-1.667607	-0.240828	1.555969
H	-1.561664	-0.321193	0.532579
O	0.202217	1.373761	1.923613
H	-0.432749	2.043453	2.241812

(H₂SO₄)₂(CH₃NH₂)(H₂O)- A 0.00 kcal/mol

C	3.323479	-0.048941	-0.801372
N	2.308666	-1.117928	-0.604272
H	2.791568	0.901123	-0.887888
H	4.001147	-0.021979	0.055539
H	3.884603	-0.240545	-1.719339
H	1.592248	-1.114275	-1.392418
H	2.736386	-2.045190	-0.549738
S	-0.504200	0.161362	-2.074792
O	0.172169	1.069023	-1.117999
O	0.350535	-0.972145	-2.455692
O	-1.875982	-0.181205	-1.687251
H	1.753627	-0.959000	0.283443
O	-0.624570	0.978731	-3.466551
H	-1.335918	1.637305	-3.362159
S	0.084162	0.208643	2.351485
O	0.741840	-0.842527	1.560292
O	0.683983	0.625560	3.581581
O	-0.073286	1.482412	1.434183
H	-0.058119	1.252692	0.444119
O	-1.370253	-0.253292	2.655972
H	-1.850814	-0.650878	1.818644
O	-2.626641	-1.236973	0.669679
H	-3.573610	-1.045754	0.740067
H	-2.344407	-0.871109	-0.212934

(H₂SO₄)₂(CH₃NH₂)(H₂O)- B 0.01 kcal/mol

C	3.325015	-0.045263	-0.795329
N	2.311024	-1.115685	-0.602191
H	2.792461	0.904677	-0.879289
H	4.002245	-0.020267	0.062003
H	3.886854	-0.233508	-1.713561
H	1.594888	-1.110344	-1.390857
H	2.739473	-2.042762	-0.550435
S	-0.503109	0.159839	-2.075261
O	0.170779	1.069363	-1.118565
O	0.353502	-0.973259	-2.453526
O	-1.875136	-0.183901	-1.689633
H	1.755000	-0.960054	0.285597

O	-0.622280	0.975382	-3.468109
H	-1.335336	1.632479	-3.366087
S	0.083613	0.206811	2.350520
O	0.736865	-0.845731	1.557442
O	0.686141	0.620629	3.580363
O	-0.070384	1.482123	1.434465
H	-0.057480	1.252912	0.444279
O	-1.372013	-0.250553	2.655827
H	-1.854676	-0.645498	1.818276
O	-2.633734	-1.227527	0.669997
H	-3.579384	-1.029885	0.740466
H	-2.349292	-0.864985	-0.213313

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})$ - C 2.45 kcal/mol

C	3.766233	-0.770885	0.132069
N	2.335608	-0.427843	-0.031099
H	3.902092	-1.853135	0.057283
H	4.350770	-0.275379	-0.647425
H	4.108507	-0.428999	1.112299
H	1.722935	-0.843298	0.706745
H	2.135322	0.625756	0.028306
S	-0.660124	-0.062600	2.075563
O	-1.806593	-0.094092	1.097531
O	0.325102	-1.109386	1.772265
O	-0.133020	1.268594	2.310861
H	1.937760	-0.722940	-0.944251
O	-1.353376	-0.439776	3.479567
H	-1.772439	-1.315398	3.384936
S	-0.580177	-0.056217	-2.121522
O	0.699876	-0.712088	-2.332186
O	-1.316710	-0.236456	-3.537398
O	-1.477639	-0.848264	-1.177524
H	-1.580982	-0.455620	-0.090691
O	-0.561034	1.358179	-1.777259
H	-2.184581	0.207092	-3.489389
O	1.447474	2.118658	0.126088
H	0.782619	2.099950	-0.595245
H	0.903517	2.040302	0.942492

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})$ - D 3.04 kcal/mol

C	3.217848	1.114552	0.592259
N	2.516355	-0.081814	0.057133
H	2.460778	1.816979	0.947249
H	3.863997	0.823259	1.424182
H	3.810391	1.577631	-0.200623
H	1.877267	0.185086	-0.757390
H	3.173241	-0.790458	-0.277912
S	-0.288098	-0.114626	-2.304487
O	-0.813763	0.071997	-3.633351
O	0.920836	0.649872	-1.955695
O	-1.334626	-0.015723	-1.233952
H	1.902919	-0.523111	0.800796

O	0.259563	-1.655810	-2.178029
H	-0.393564	-2.234583	-2.612152
S	-0.380121	-0.429688	2.175773
O	-0.952315	-0.498208	3.487146
O	0.884953	-1.135066	1.950870
O	-1.474519	-0.935942	1.166893
H	-1.283605	-0.671413	0.195785
O	-0.091832	1.050959	1.717184
H	-0.911721	1.513555	1.262843
O	-1.908177	2.133980	0.321479
H	-1.821533	1.497508	-0.434904
H	-2.829197	2.071480	0.617685

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})$ - E 3.18 kcal/mol

C	3.243080	0.052962	0.781358
N	2.281738	1.153081	0.491277
H	2.670264	-0.865990	0.924691
H	3.936483	-0.054692	-0.056338
H	3.790911	0.280093	1.699062
H	1.518636	1.211187	1.228251
H	2.749413	2.060025	0.425027
S	-0.406859	-0.246325	2.091982
O	0.600293	-1.276151	2.281481
O	0.091085	1.140187	2.093826
O	-1.291711	-0.525933	0.914919
H	1.756823	0.987149	-0.415760
O	-1.399709	-0.242076	3.369367
H	-1.726348	-1.152939	3.491801
S	0.036788	-0.241584	-2.331905
O	0.701105	0.887236	-1.657866
O	0.647681	-0.797341	-3.498491
O	-0.123587	-1.413426	-1.286378
H	-0.554447	-1.096383	-0.421701
O	-1.414267	0.207125	-2.681982
H	-1.856497	0.711444	-1.881675
O	-2.497506	1.318119	-0.647469
H	-2.159184	2.208176	-0.466299
H	-2.142630	0.747203	0.085382

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})$ - F 3.21 kcal/mol

C	2.885302	0.920359	-0.934593
N	2.348605	-0.457839	-1.095407
H	2.038700	1.585250	-0.749663
H	3.577482	0.954697	-0.089529
H	3.393717	1.221328	-1.853822
H	1.628846	-0.483271	-1.902077
H	3.090668	-1.133233	-1.291959
S	-0.707583	0.201798	-2.507116
O	-1.382596	1.110889	-3.404095
O	0.547557	-0.388755	-3.030672
O	-0.479075	0.707653	-1.122363
H	1.852674	-0.758581	-0.221023

O	-1.714632	-1.059869	-2.256639
H	-2.374708	-1.031103	-2.971909
S	-0.001091	-0.544883	1.962470
O	-0.491326	-1.163747	3.174834
O	1.069000	-1.208851	1.231065
O	-1.224792	-0.300912	1.043846
H	-0.949067	0.094081	0.104744
O	0.559492	0.899631	2.297527
H	0.024830	1.253931	3.088520
O	-0.873488	1.326404	4.452894
H	-1.749434	1.731160	4.358425
H	-1.028071	0.358273	4.426858

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})$ - G 3.29 kcal/mol

C	2.884812	0.919425	-0.942266
N	2.348889	-0.459682	-1.097968
H	2.038113	1.584058	-0.756806
H	3.579254	0.956659	-0.099166
H	3.390517	1.218422	-1.863640
H	1.626429	-0.487913	-1.902668
H	3.091048	-1.134721	-1.295335
S	-0.708073	0.201333	-2.507269
O	-1.376004	1.114965	-3.404840
O	0.544205	-0.396971	-3.029197
O	-0.478210	0.705371	-1.122144
H	1.856104	-0.758741	-0.221245
O	-1.723344	-1.054130	-2.258936
H	-2.382260	-1.020804	-2.975095
S	-0.000317	-0.542984	1.963196
O	-0.489455	-1.163415	3.175320
O	1.072658	-1.203432	1.232926
O	-1.224271	-0.303819	1.043651
H	-0.949099	0.090153	0.103902
O	0.554783	0.903592	2.298348
H	0.020689	1.255433	3.090934
O	-0.870117	1.321346	4.459997
H	-1.747656	1.724203	4.372644
H	-1.021936	0.352819	4.430010

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})$ - H 3.64 kcal/mol

C	3.477960	-0.194773	0.158918
N	2.055183	0.144615	-0.084164
H	4.111839	0.353964	-0.542177
H	3.748968	0.059405	1.186823
H	3.611389	-1.267936	0.003392
H	1.747097	-0.095778	-1.078899
H	1.417708	-0.354517	0.590190
S	-0.183986	0.108600	-2.680118
O	-0.580818	0.611657	-3.973601
O	1.210425	-0.369079	-2.581665
O	-0.521131	0.953892	-1.500302
H	1.867001	1.142229	0.050198

O	-1.134063	-1.219037	-2.386799
H	-1.372736	-1.580745	-3.258865
S	-0.310894	-0.130546	2.673938
O	-0.146269	-0.364352	4.083769
O	0.368189	-1.019651	1.727320
O	-1.759709	0.069497	2.305852
H	-2.048438	0.067362	1.084626
O	0.405432	1.312579	2.319238
H	0.145651	1.944226	3.014657
O	-2.394405	0.093384	-0.032361
H	-1.655043	0.503578	-0.639805
H	-2.490605	-0.815437	-0.367228

(H₂SO₄)₂(CH₃NH₂)(H₂O)- I 3.65 kcal/mol

C	3.478166	-0.191541	0.160265
N	2.055206	0.146175	-0.084488
H	4.112057	0.356959	-0.541012
H	3.748024	0.064224	1.188080
H	3.612731	-1.264778	0.006203
H	1.748289	-0.095292	-1.079467
H	1.417776	-0.353135	0.589593
S	-0.183742	0.107492	-2.679907
O	-0.579486	0.609225	-3.974222
O	1.210402	-0.371405	-2.580740
O	-0.520736	0.954275	-1.501201
H	1.865979	1.143686	0.049109
O	-1.135388	-1.218528	-2.384249
H	-1.363958	-1.589663	-3.255091
S	-0.311079	-0.131782	2.673252
O	-0.148604	-0.368951	4.082793
O	0.366953	-1.020491	1.725550
O	-1.759050	0.073134	2.304278
H	-2.048879	0.071950	1.083374
O	0.409384	1.310438	2.322021
H	0.145511	1.943056	3.015044
O	-2.396489	0.099687	-0.033112
H	-1.655760	0.507400	-0.640582
H	-2.495964	-0.808803	-0.367899

(H₂SO₄)₂(CH₃NH₂)(H₂O)- J 4.15 kcal/mol

C	2.880684	0.931457	-0.933943
N	2.352440	-0.450123	-1.093691
H	2.030163	1.591111	-0.748304
H	3.573538	0.970348	-0.089631
H	3.386219	1.235282	-1.853817
H	1.631243	-0.480607	-1.898776
H	3.098442	-1.120765	-1.291539
S	-0.708201	0.197922	-2.507055
O	-1.376900	1.111850	-3.404080
O	0.546574	-0.397437	-3.024736
O	-0.483449	0.703064	-1.120927
H	1.859974	-0.753872	-0.218339

O	-1.719646	-1.062661	-2.269217
H	-2.410452	-0.991293	-2.951671
S	0.006464	-0.545566	1.965122
O	-0.480095	-1.165448	3.178342
O	1.085266	-1.200853	1.238631
O	-1.217527	-0.317381	1.042835
H	-0.944932	0.081827	0.104025
O	0.551366	0.905870	2.296358
H	0.009218	1.258256	3.083040
O	-0.897737	1.329264	4.441949
H	-1.042463	0.359571	4.422719
H	-1.777163	1.724410	4.339465

(H₂SO₄)₂(CH₃NH₂)(H₂O)- K 6.03 kcal/mol

C	3.379566	-1.013107	-0.416187
N	2.042157	-0.395234	-0.582736
H	4.045643	-0.297498	0.072038
H	3.294671	-1.907795	0.205477
H	3.784800	-1.280148	-1.395779
H	0.912590	1.460256	-2.640208
H	1.369448	-1.030262	-1.048266
S	-1.186749	-0.078610	-1.953371
O	-2.561444	-0.478786	-2.127552
O	-0.577945	0.687727	-3.045088
O	-0.813622	0.494484	-0.632827
H	1.621799	-0.158917	0.344352
O	-0.302545	-1.512578	-1.873598
H	-0.644525	-2.099126	-2.571323
S	-0.223485	0.009116	2.633904
O	-0.493910	-0.615824	3.896276
O	1.077603	-0.160958	2.006126
O	-1.368067	-0.355948	1.654911
H	-1.183383	-0.019809	0.670079
O	-0.336053	1.612022	2.792997
H	-1.127050	1.805810	3.330941
O	1.813215	1.716739	-2.297225
H	2.346572	1.917781	-3.078997
H	2.072839	0.471855	-1.192738

(H₂SO₄)₂(CH₃NH₂)(H₂O)- L 6.84 kcal/mol

C	3.492612	-0.152806	0.377786
N	2.235911	-0.948589	0.432770
H	3.204029	0.897644	0.296421
H	4.066374	-0.323226	1.292167
H	4.078339	-0.454788	-0.494340
H	1.646166	-0.801072	-0.419650
H	2.421796	-1.952698	0.500343
S	-0.443693	-0.063336	-2.255548
O	-0.129194	1.296382	-2.645560
O	0.642056	-0.943265	-1.847131
O	-1.594358	-0.092776	-1.246597
H	1.642307	-0.676208	1.271404
O	-1.077851	-0.796815	-3.539362

H	-1.517711	-0.114884	-4.080332
S	-0.680409	-0.010110	2.117685
O	-1.572159	-0.485807	3.377638
O	0.681849	-0.317049	2.567015
O	-1.081105	-0.919811	0.989812
H	-1.336479	-0.438302	-0.223256
O	-0.990204	1.388494	1.858495
H	-2.459500	-0.095337	3.272283
O	1.174668	1.943281	-0.038394
H	0.440778	2.040360	0.599200
H	0.762882	2.069520	-0.911853

(H₂SO₄)₂(CH₃NH₂)(H₂O)- M 7.49 kcal/mol

C	3.498401	-0.191343	0.381495
N	2.228985	-0.967369	0.429707
H	3.226310	0.864037	0.308645
H	4.068434	-0.378426	1.294979
H	4.080142	-0.495795	-0.492470
H	1.642002	-0.806741	-0.421873
H	2.400090	-1.974467	0.491563
S	-0.442819	-0.034924	-2.263062
O	-0.074941	1.315706	-2.600165
O	0.614923	-0.958445	-1.850816
O	-1.620742	-0.099532	-1.276932
H	1.637626	-0.692365	1.270282
O	-1.106218	-0.608739	-3.607075
H	-1.419722	-1.516723	-3.435832
S	-0.685875	-0.009200	2.109252
O	-1.587824	-0.482600	3.363970
O	0.671708	-0.338888	2.558434
O	-1.095072	-0.902005	0.973033
H	-1.355616	-0.415153	-0.254777
O	-0.976672	1.396322	1.864772
H	-2.454960	-0.044547	3.280305
O	1.217985	1.926949	-0.003348
H	0.481767	2.039832	0.628698
H	0.814551	2.055834	-0.880462

(H₂SO₄)₂(CH₃NH₂)(H₂O)- N 8.22 kcal/mol

C	3.498515	-0.227416	0.455421
N	2.209186	-0.971031	0.474324
H	3.254490	0.835435	0.394814
H	4.052223	-0.444410	1.372392
H	4.083120	-0.532456	-0.416449
H	1.634216	-0.775336	-0.377238
H	2.354753	-1.983425	0.509061
S	-0.427924	-0.035524	-2.268902
O	-0.058587	1.318079	-2.589958
O	0.622587	-0.955271	-1.832575
O	-1.633394	-0.112587	-1.312983
H	1.614566	-0.705214	1.316822
O	-1.059300	-0.605310	-3.629049

H	-1.388755	-1.509031	-3.465270
S	-0.716895	0.015444	2.091508
O	-1.754924	-0.313408	3.284809
O	0.615559	-0.381154	2.593272
O	-1.109365	-0.887514	0.959033
H	-1.384753	-0.409881	-0.293473
O	-0.921368	1.424662	1.831360
H	-1.580813	-1.220911	3.595000
O	1.275327	1.908436	-0.003217
H	0.534573	2.017316	0.625320
H	0.875808	2.043441	-0.881001

(H₂SO₄)₂(CH₃NH₂)(H₂O)₂- A 0.00 kcal/mol

C	3.179811	0.958887	-0.527139
N	2.597536	-0.379593	-0.238112
H	3.811329	0.900448	-1.417144
H	2.353280	1.648169	-0.713501
H	3.763832	1.296680	0.332316
H	-0.801053	-0.426568	4.471550
H	2.042540	-0.346319	0.668313
S	0.016975	-0.130314	2.530118
O	1.438132	-0.150527	2.159340
O	0.097226	-0.510308	4.102266
O	-0.624348	1.187523	2.450297
H	1.958868	-0.680985	-1.033084
O	-0.769599	-1.206606	1.884904
H	3.325091	-1.089599	-0.125854
S	-0.188473	-0.208827	-2.444697
O	-0.074385	1.060620	-1.704589
O	0.999030	-1.061682	-2.303102
O	-1.473679	-0.903585	-2.226541
H	-2.153947	-0.839274	-0.795572
O	-0.161333	0.144021	-4.025774
H	-1.036336	0.501351	-4.264030
O	-2.548852	-0.596106	0.112886
H	-1.887202	-0.921158	0.823950
H	-2.413718	0.490847	0.142999
O	-1.973862	1.816056	0.163903
H	-1.288631	1.764298	-0.547845
H	-1.458331	1.796924	1.012052

(H₂SO₄)₂(CH₃NH₂)(H₂O)₂- B 3.10 kcal/mol

C	-2.363047	2.166065	0.137404
N	-2.642128	0.719876	0.348640
H	-1.291094	2.277875	-0.037769
H	-2.911386	2.523715	-0.737411
H	-2.656322	2.728712	1.027038
H	-2.118434	0.365378	1.210305
H	-3.639997	0.545604	0.489550
S	0.130287	-0.264664	2.447696
O	0.962988	0.422628	3.410675
O	-1.323010	-0.055042	2.540892

O	0.599824	-0.063136	1.035411
H	-2.323233	0.157398	-0.491985
O	0.265153	-1.860843	2.727518
H	1.160915	-2.015144	3.079248
S	-0.400684	-0.627332	-2.252029
O	-0.072341	-1.181713	-3.533431
O	-1.804149	-0.648405	-1.832137
O	0.481767	-1.393959	-1.192091
H	0.436003	-0.947769	-0.278331
O	0.037876	0.867511	-2.110786
H	1.091156	0.990089	-2.208460
O	2.518421	1.236275	-2.186869
H	2.809507	1.130562	-1.225393
H	2.993621	0.560123	-2.693678
O	3.070683	0.890357	0.366457
H	2.213158	0.571242	0.747583
H	3.337957	1.639246	0.918629

(H₂SO₄)₂(CH₃NH₂)(H₂O)₂- C 4.07 kcal/mol

C	3.180627	-1.879618	-0.494639
N	2.145401	-0.823903	-0.394301
H	3.767369	-1.726340	-1.403877
H	3.836642	-1.837138	0.378838
H	2.696157	-2.858263	-0.537590
H	1.486003	-0.847801	-1.219621
H	1.567687	-0.918355	0.469253
S	-0.807546	-0.038578	-2.312231
O	-1.045617	1.042360	-3.241696
O	0.404162	-0.843467	-2.496430
O	-0.934643	0.407941	-0.873341
H	2.555924	0.140302	-0.338823
O	-1.993475	-1.131412	-2.493852
H	-2.793524	-0.644547	-2.764534
S	-0.631624	-0.356228	2.456039
O	-1.068910	-0.937576	3.684612
O	0.722475	-0.623153	1.971907
O	-1.662200	-0.767915	1.339926
H	-1.387684	-0.402941	0.430549
O	-0.795389	1.214028	2.598586
H	-0.398422	1.694293	1.807184
O	0.141586	2.426013	0.367901
H	-0.290188	1.771790	-0.266412
H	-0.252958	3.290446	0.175260
O	2.834509	1.877378	-0.110417
H	3.390596	2.174705	0.624450
H	1.927566	2.212184	0.094761

(H₂SO₄)₂(CH₃NH₂)(H₂O)₂- D 5.90 kcal/mol

C	3.619655	-0.920994	-0.413104
N	2.201465	-0.496941	-0.495252
H	4.158900	-0.232124	0.241567
H	3.681707	-1.932273	-0.002876

H	4.066858	-0.897749	-1.410223
H	1.041987	1.646124	-2.202122
H	1.635154	-1.113720	-1.100787
S	-1.025376	-0.303549	-2.161806
O	-2.252240	-0.828331	-2.708299
O	-0.287464	0.665420	-2.971510
O	-1.086938	0.134483	-0.731110
H	1.740291	-0.491174	0.446149
O	-0.009373	-1.626647	-2.003146
H	-0.289001	-2.270198	-2.678247
S	-0.305619	-0.280047	2.605511
O	-0.461579	-0.861075	3.899726
O	1.008067	-0.308692	1.960768
O	-1.357105	-0.969026	1.652149
H	-1.275507	-0.639380	0.700155
O	-0.767454	1.225818	2.702217
H	-0.581062	1.728429	1.842090
O	1.728626	1.955508	-1.560920
H	1.208049	2.437078	-0.887253
H	2.093845	0.492183	-0.893341
O	-0.444428	2.455781	0.352273
H	-0.788681	1.692983	-0.195628
H	-1.085702	3.176004	0.249458

(H₂SO₄)₂(CH₃NH₂)(H₂O)₂- E 6.03 kcal/mol

C	3.595770	-0.975291	-0.451879
N	2.186870	-0.518332	-0.515060
H	4.163757	-0.290752	0.182694
H	3.640490	-1.982007	-0.028491
H	4.024628	-0.976962	-1.457301
H	1.062201	1.634316	-2.223216
H	1.598900	-1.125523	-1.110102
S	-1.042444	-0.292964	-2.149267
O	-2.281307	-0.794341	-2.690545
O	-0.280120	0.647140	-2.970120
O	-1.094259	0.163258	-0.723896
H	1.737555	-0.501937	0.431766
O	-0.059298	-1.638723	-1.972754
H	-0.351742	-2.282825	-2.641934
S	-0.300060	-0.276576	2.607213
O	-0.464807	-0.852211	3.902724
O	1.006073	-0.350383	1.951271
O	-1.383496	-0.927585	1.663374
H	-1.296895	-0.603457	0.709958
O	-0.708904	1.244741	2.708842
H	-0.515758	1.740181	1.846654
O	1.758282	1.939072	-1.590494
H	1.250274	2.430611	-0.914298
H	2.097320	0.470950	-0.916395
O	-0.375448	2.465266	0.351924
H	-0.744832	1.710844	-0.191427
H	-1.002273	3.199427	0.259041

$(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_2$ - F 6.63 kcal/mol

C	3.579463	0.061948	-1.946854
N	2.212152	0.093098	-1.378067
H	3.804711	1.012965	-2.436846
H	4.301928	-0.118336	-1.146460
H	3.644199	-0.747689	-2.677892
H	1.458216	0.272420	-2.090350
H	1.929214	-0.846823	-0.938951
S	-1.284724	0.156113	-1.989337
O	-2.571457	0.424781	-2.582279
O	-0.104234	0.414073	-2.826176
O	-1.081992	0.703257	-0.611143
H	2.094721	0.832358	-0.665604
O	-1.260182	-1.476268	-1.684356
H	-1.995837	-1.862510	-2.192192
S	-0.171042	-0.160646	2.647366
O	-0.443824	-0.623699	3.970141
O	0.906499	-0.754472	1.861053
O	-1.521571	-0.271562	1.832786
H	-1.399721	0.020085	0.875912
O	0.115024	1.395802	2.736220
H	0.491263	1.722359	1.861068
O	0.905352	2.178265	0.276271
H	0.110125	1.774441	-0.182454
H	0.854135	3.134223	0.124838
O	1.256649	-2.233384	-0.398427
H	0.386980	-2.260208	-0.843960
H	1.048360	-1.938473	0.519308

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_2$ - G 6.84 kcal/mol

C	3.065431	0.042738	0.537971
N	1.631635	0.174518	0.180643
H	3.194769	0.296068	1.592540
H	3.378762	-0.990460	0.370577
H	3.661300	0.709846	-0.089916
H	-0.764174	1.493498	-4.171692
H	1.441604	-0.094157	-0.815250
S	-0.092871	-0.329155	-3.287958
O	1.060464	-0.515729	-2.415295
O	-0.161508	1.292338	-3.431328
O	-0.075047	-0.910848	-4.599790
H	1.009870	-0.415746	0.791672
O	-1.399907	-0.691551	-2.577733
H	-1.523560	-0.280305	-1.537603
S	-0.446776	-0.342049	3.047390
O	-0.381058	-0.965803	1.692200
O	-1.119722	-1.108340	4.067230
O	1.164048	-0.343632	3.428120
H	1.215400	-0.341061	4.400665
O	-0.828452	1.082767	2.968357
H	-0.486522	1.898335	1.621033

O	-1.788477	0.181623	-0.329715
H	-1.445690	-0.384929	0.413140
H	-1.384067	1.066511	-0.141972
O	-0.262135	2.226897	0.689357
H	1.264659	1.138178	0.308880
H	-0.407691	3.183664	0.683452

(H₂SO₄)₂(CH₃NH₂)(H₂O)₂- H 8.47 kcal/mol

C	3.265199	1.281960	-0.163949
N	2.786247	-0.105499	-0.403630
H	2.419961	1.870340	0.199297
H	4.048720	1.272444	0.597897
H	3.648321	1.706451	-1.095244
H	2.068630	-0.130438	-1.188224
H	3.554251	-0.726024	-0.670110
S	-0.400388	-0.110673	-2.483270
O	-0.992055	0.851931	-3.384289
O	1.075660	-0.132513	-2.471669
O	-0.959276	-0.090507	-1.097130
H	2.328206	-0.501142	0.478557
O	-0.866576	-1.597730	-2.958731
H	-0.808599	-1.615054	-3.931348
S	0.377029	-0.368161	2.221010
O	-0.002243	-0.502101	3.600685
O	1.615725	-1.054272	1.807124
O	-0.845431	-1.096310	1.405206
H	-0.748257	-0.915927	0.427370
O	0.391438	1.043182	1.691181
H	-0.766562	1.543190	1.105844
O	-1.646909	1.792622	0.516846
H	-1.479883	1.217508	-0.304224
H	-2.413012	1.321215	1.010182
O	-3.261703	0.306966	1.883699
H	-4.052853	-0.094535	1.494233
H	-2.589150	-0.410089	1.937650

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- A 0.00 kcal/mol

C	3.727476	-0.288900	0.007059
N	2.248928	-0.191992	-0.017197
H	4.113637	0.215022	0.896644
H	4.011620	-1.343577	0.035938
H	4.140382	0.174722	-0.892481
H	0.439313	-0.047021	-4.779740
H	1.829811	-0.639146	-0.881223
S	0.126416	0.048789	-2.675254
O	1.000823	-1.073026	-2.270739
O	0.693254	0.597512	-4.093958
O	-1.259303	-0.364194	-2.937039
H	1.808165	-0.618990	0.845285
O	0.282675	1.222612	-1.803342
H	1.924235	0.781456	-0.046591
S	0.102552	-0.098247	2.711016

O	-1.318309	-0.495418	2.777309
O	1.006442	-1.142846	2.213015
O	0.315901	1.207942	2.058724
H	-0.805377	1.943515	0.859481
O	0.575693	0.056062	4.252588
H	-0.085275	0.605878	4.712298
O	-1.465250	2.052142	0.129338
H	-0.944227	1.839842	-0.686850
H	-2.322904	0.981665	0.421762
O	-2.874176	0.113751	0.781235
H	-2.324483	-0.192940	1.580137
H	-2.828043	-0.623158	0.052161
O	-2.736561	-1.615566	-1.096308
H	-2.173866	-1.216222	-1.819226
H	-2.323354	-2.464123	-0.878346

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- B 0.01 kcal/mol

C	3.725764	-0.292010	0.005929
N	2.247278	-0.194175	-0.019005
H	4.111877	0.212942	0.894948
H	4.009258	-1.346816	0.036434
H	4.139310	0.170082	-0.894103
H	0.436258	-0.043044	-4.780759
H	1.828152	-0.642678	-0.882213
S	0.126012	0.049961	-2.675782
O	0.998580	-1.073952	-2.273173
O	0.693130	0.599551	-4.094237
O	-1.260589	-0.359991	-2.937284
H	1.806077	-0.619229	0.844324
O	0.284998	1.222428	-1.802421
H	1.923246	0.779449	-0.050730
S	0.102842	-0.096896	2.712052
O	-1.318136	-0.493675	2.778850
O	1.006240	-1.141450	2.213052
O	0.316313	1.209466	2.060368
H	-0.806238	1.943386	0.861028
O	0.576401	0.056303	4.253691
H	-0.086127	0.603277	4.714548
O	-1.465144	2.050158	0.129706
H	-0.942961	1.836686	-0.685440
H	-2.321553	0.979056	0.422323
O	-2.873022	0.110943	0.781323
H	-2.323659	-0.195492	1.580720
H	-2.826251	-0.625829	0.052394
O	-2.734156	-1.618169	-1.096937
H	-2.173355	-1.216894	-1.820095
H	-2.318137	-2.465548	-0.879724

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- C 0.55 kcal/mol

C	3.518820	0.292290	-0.814137
N	2.589267	-0.720964	-0.246952
H	4.018018	-0.118378	-1.695320

H	2.924600	1.161874	-1.103761
H	4.254906	0.577612	-0.058643
H	-0.193840	-0.053926	4.592435
H	2.133377	-0.337694	0.636557
S	0.340735	0.074007	2.537422
O	1.678015	0.391412	2.013261
O	0.645967	-0.175585	4.113375
O	-0.624702	1.181080	2.499301
H	1.844670	-0.965657	-0.962848
O	-0.183918	-1.192224	1.990690
H	3.079875	-1.581184	0.008324
S	-0.061787	-0.110215	-2.507562
O	0.269406	1.070133	-1.704080
O	0.805048	-1.269488	-2.215575
O	-1.490866	-0.470202	-2.558289
H	-2.507189	-0.098913	-1.370321
O	0.313478	0.372311	-4.013864
H	-0.030038	-0.299206	-4.631309
O	-3.032250	0.217206	-0.563930
H	-1.781781	-1.436707	1.592357
H	-2.435124	1.082096	-0.206353
O	-1.560415	2.072016	0.125841
H	-0.829494	1.906588	-0.518573
H	-1.183680	1.834823	1.017589
O	-2.724991	-1.546993	1.274026
H	-2.802951	-2.471761	0.997667
H	-2.950502	-0.524571	0.151881

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- D 1.36 kcal/mol

C	3.787405	-1.092899	-0.328004
N	2.462245	-0.435156	-0.232817
H	4.337489	-0.944263	0.604574
H	3.650803	-2.161793	-0.510024
H	4.345720	-0.653191	-1.158068
H	-0.517871	-0.033340	-4.679300
H	1.904150	-0.551566	-1.123988
S	-0.245399	-0.042943	-2.567345
O	1.049653	-0.745549	-2.541799
O	-0.352485	0.667754	-4.022350
O	-1.401995	-0.938233	-2.463126
H	1.905617	-0.793005	0.564496
O	-0.266896	1.119412	-1.655549
H	2.540822	0.588991	-0.009101
S	-0.344649	-0.200850	2.481523
O	-1.060104	-1.315835	1.852688
O	1.105440	-0.195023	2.238987
O	-0.976464	1.119683	2.246739
H	-1.758744	1.376686	0.902780
O	-0.406288	-0.436100	4.082775
H	-1.344926	-0.465385	4.344751
O	-2.243024	1.396302	0.003279
H	-1.502577	1.398588	-0.698200

H	-2.642910	0.367473	-0.081357
O	-2.889071	-0.980904	-0.177866
H	-2.293376	-1.308088	0.542019
H	-2.414059	-1.178829	-1.025680
O	2.392300	2.011545	1.046854
H	1.840128	1.512600	1.689953
H	1.821828	2.724873	0.722984

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- E 1.93 kcal/mol

C	3.334460	1.102436	-0.893414
N	2.820371	-0.212994	-0.426237
H	3.863027	0.974308	-1.841389
H	2.475296	1.759993	-1.042740
H	4.004310	1.523573	-0.139667
H	0.759294	-0.069365	4.509003
H	2.346581	-0.105098	0.520865
S	0.438830	-0.167647	2.406357
O	1.811110	0.222009	2.022046
O	0.555382	-0.800791	3.897776
O	-0.483639	0.964553	2.511995
H	2.123358	-0.600449	-1.131262
O	-0.054646	-1.317504	1.628457
H	3.574827	-0.894709	-0.317562
S	-0.104272	-0.235608	-2.390734
O	0.027482	1.009983	-1.635087
O	1.105389	-1.081241	-2.320899
O	-1.344837	-1.000664	-2.153097
H	-1.860815	-1.327876	-0.721241
O	-0.220634	0.275186	-3.925987
H	-0.494824	-0.485718	-4.470218
O	-2.215612	-1.454211	0.230271
H	-1.401383	-1.396575	0.845491
H	-2.857369	-0.606546	0.428550
O	-3.611153	0.572789	0.561322
H	-2.889487	1.301988	0.453971
H	-3.992387	0.689587	1.444269
O	-1.634880	2.205731	0.301933
H	-1.118304	1.888545	-0.472900
H	-1.106111	1.910049	1.079150

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- F 2.00 kcal/mol

C	3.194662	1.525548	-0.560621
N	2.416188	0.309732	-0.220916
H	4.044762	1.246522	-1.187970
H	2.547548	2.215101	-1.108064
H	3.552127	1.998313	0.357517
H	-1.435717	-0.273506	4.318914
H	1.619877	0.532554	0.407241
S	-0.536077	0.082157	2.419574
O	0.894125	0.290284	2.140977
O	-0.515034	-0.146463	4.024562
O	-1.377670	1.254942	2.165310

H	2.025921	-0.148345	-1.088903
O	-1.070072	-1.169802	1.839480
H	2.961685	-0.383629	0.337412
S	-0.094338	-0.241644	-2.567725
O	-0.287394	1.007698	-1.822253
O	1.276310	-0.771769	-2.460896
O	-1.123404	-1.275337	-2.334217
H	-2.056036	-1.218612	-1.058701
O	-0.290024	0.225438	-4.108886
H	-0.291558	-0.576221	-4.663836
O	-2.629326	-1.002556	-0.243084
H	-2.047466	-1.162635	0.577531
H	-2.699182	0.099995	-0.280212
O	-2.533795	1.467468	-0.302797
H	-1.767298	1.526056	-0.927297
H	-2.136334	1.602552	0.596080
O	3.183752	-1.265637	1.935881
H	3.136572	-2.226077	2.046781
H	2.330712	-0.915814	2.281446

(H₂SO₄)₂(CH₃NH₂)(H₂O)₃- G 3.11 kcal/mol

C	3.332772	0.774671	0.380439
N	2.640023	-0.538095	0.482237
H	4.030009	0.755993	-0.460918
H	2.573281	1.538952	0.202302
H	3.865684	0.982341	1.311525
H	-0.373134	-0.184883	4.926263
H	1.993959	-0.548434	1.326540
S	-0.287275	-0.276887	2.801149
O	1.175866	-0.464831	2.739012
O	-0.735286	-0.805440	4.267464
O	-0.688459	1.134218	2.729231
H	2.077067	-0.720031	-0.405513
O	-1.022959	-1.186748	1.909866
H	3.306633	-1.305526	0.594700
S	0.269388	0.089294	-2.094291
O	0.355119	1.240051	-1.186964
O	1.334796	-0.902155	-1.840531
O	-1.080886	-0.550390	-2.131321
H	-2.017581	-0.458991	-0.826752
O	0.502939	0.673784	-3.550460
H	-0.024433	0.114217	-4.208175
O	-2.529824	-0.238106	0.022124
H	-2.024000	-0.693825	0.780793
H	-2.277022	0.836076	0.185386
O	-1.724850	2.060270	0.400879
H	-0.958018	1.999867	-0.223802
H	-1.322375	1.910457	1.297981
O	-1.173974	-0.875882	-4.891702
H	-1.498203	-1.061262	-3.983303
H	-0.842310	-1.722988	-5.225834

$(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_4$ - A 0.00 kcal/mol

C	3.806809	-1.336242	-0.093363
N	2.474624	-0.693068	-0.063575
H	4.358398	-1.076259	0.813946
H	3.691656	-2.422047	-0.148418
H	4.360555	-0.986025	-0.968426
H	0.249784	-0.009333	-4.770162
H	1.910083	-0.896834	-0.924641
S	-0.058039	0.071368	-2.663549
O	0.893941	-0.998731	-2.317438
O	0.414593	0.673354	-4.094015
O	-1.428756	-0.418662	-2.866358
H	1.909486	-0.975991	0.769667
O	0.039554	1.256040	-1.793185
H	2.518722	0.366969	-0.004632
S	-0.049084	-0.104418	2.691943
O	-1.457333	-0.531639	2.807443
O	0.851587	-1.120296	2.150796
O	0.085502	1.230861	2.064330
H	-1.158502	1.840901	0.864731
O	0.482849	0.051422	4.213331
H	-0.127176	0.649220	4.683747
O	-1.821726	1.886692	0.133534
H	-1.280815	1.722564	-0.679735
H	-2.597848	0.737570	0.432214
O	-3.061108	-0.167100	0.800980
H	-2.481934	-0.399654	1.605410
H	-2.938882	-0.905221	0.078595
O	-2.745052	-1.874795	-1.066124
H	-2.226567	-1.402654	-1.779481
H	-2.237608	-2.671594	-0.852155
O	2.078029	2.000420	0.114349
H	1.486957	1.924239	0.894129
H	1.457783	2.001348	-0.645041

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_4$ - B 0.33 kcal/mol

C	3.746114	0.291887	0.111232
N	2.294830	0.078295	-0.095185
H	3.914751	0.715324	1.104636
H	4.259330	-0.669657	0.033857
H	4.130394	0.970991	-0.654219
H	0.396081	0.246145	-4.912310
H	2.068388	-0.310461	-1.054573
S	0.227914	0.016903	-2.801912
O	1.465830	-0.747731	-2.543772
O	0.479293	0.865099	-4.163916
O	-0.937019	-0.832559	-3.077197
H	1.880450	-0.555693	0.642782
O	0.015816	1.077898	-1.803115
H	1.761603	0.952186	-0.024183
S	0.258408	-0.413312	2.642212
O	-1.186163	-0.689833	2.697095

O	1.047483	-1.367004	1.850253
O	0.577766	0.990891	2.309515
H	-0.642388	2.207965	2.026990
O	0.799344	-0.677353	4.148849
H	0.145968	-0.298515	4.765144
O	-1.357624	2.824770	1.724711
H	-0.956434	3.704274	1.685148
H	-2.176977	-0.687510	1.390894
O	-2.766719	-0.617960	0.579246
H	-2.557064	0.396590	0.100392
H	-2.485948	-1.354419	-0.078504
O	-2.056762	-2.379326	-1.172848
H	-1.619410	-1.877799	-1.913440
H	-1.407844	-3.037134	-0.882098
O	-2.278949	1.561126	-0.421637
H	-1.950893	2.140325	0.331789
H	-1.500016	1.436402	-1.025672

(H₂SO₄)₂(CH₃NH₂)(H₂O)₄- C 0.47 kcal/mol

C	3.324123	1.652433	0.704371
N	2.190832	0.885181	0.141340
H	4.229909	1.446873	0.128622
H	3.103126	2.722593	0.670950
H	3.474110	1.344504	1.742578
H	-1.118494	0.138310	4.383376
H	1.333318	1.004270	0.726365
S	-0.097661	-0.298519	2.570100
O	1.182523	-0.982062	2.454302
O	-0.176972	0.124060	4.133543
O	-0.106480	0.987592	1.802454
H	1.942093	1.137107	-0.839568
O	-1.304538	-1.098993	2.321619
H	2.382809	-0.163405	0.123373
S	0.115380	0.024314	-2.673334
O	-1.231798	0.590092	-2.871364
O	1.142370	1.048147	-2.441847
O	0.158419	-1.098953	-1.716899
H	-1.245423	-1.675717	-0.746080
O	0.497116	-0.709504	-4.066389
H	0.466053	-0.039968	-4.774412
O	-2.074302	-1.710763	-0.205671
H	-1.788447	-1.583311	0.739468
H	-2.680496	-0.571714	-0.599290
O	-3.034010	0.411700	-0.993712
H	-2.391589	0.580047	-1.758977
H	-2.829906	1.108248	-0.267223
O	-2.429973	2.025943	0.927240
H	-1.573317	1.685296	1.310592
H	-2.287751	2.962814	0.730087
O	2.360955	-1.835826	-0.004148
H	1.889190	-1.954994	0.845123
H	1.664258	-1.876015	-0.691875

$(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_4$ - D 1.43 kcal/mol

C	3.729550	-0.193225	-0.322332
N	2.299328	-0.181056	0.067496
H	4.126780	0.821387	-0.240787
H	4.285289	-0.855523	0.346169
H	3.817365	-0.542319	-1.354154
H	0.846870	-0.046572	-4.769255
H	1.873282	-1.109728	-0.024652
S	0.324401	-0.000439	-2.701220
O	0.952587	-1.266435	-2.333515
O	1.071814	0.555888	-4.036581
O	-1.103296	-0.087839	-3.041406
H	2.142449	0.137668	1.065931
O	0.625899	1.095415	-1.738255
H	1.731261	0.427705	-0.574122
S	0.359453	-0.002083	2.872346
O	0.014977	-1.076346	1.918285
O	1.677946	0.582597	2.595747
O	-0.726141	0.974638	3.075496
H	-1.863416	1.250596	1.934799
O	0.585562	-0.694768	4.321396
H	-0.291763	-0.821295	4.726367
O	-2.563427	1.199959	1.208670
H	-2.201341	1.684310	0.377893
H	-1.592725	-1.364574	1.224871
O	-2.508191	-1.221884	0.873134
H	-2.610344	0.090817	0.989469
H	-2.518761	-1.524922	-0.089082
O	-2.596583	-1.917030	-1.675421
H	-2.042676	-1.298137	-2.217956
H	-2.271649	-2.803335	-1.890104
O	-1.653634	2.377450	-0.905454
H	-2.255654	2.288332	-1.660435
H	-0.809314	1.959510	-1.218199

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_4$ - E 1.53 kcal/mol

C	3.921416	-0.227999	0.203640
N	2.465430	-0.054594	-0.013771
H	4.192521	0.158782	1.189281
H	4.161994	-1.292511	0.150415
H	4.474764	0.308750	-0.570975
H	-0.053572	-0.634682	-4.618714
H	2.142393	-0.415884	-0.954889
S	0.217813	-0.027534	-2.593657
O	1.350851	-0.939148	-2.339159
O	0.162886	0.215410	-4.192565
O	-1.077632	-0.652333	-2.231471
H	1.884266	-0.540750	0.724114
O	0.422177	1.320581	-2.065316
H	2.177670	0.929233	0.041958
S	0.166731	0.135045	2.516532

O	-1.238821	-0.003001	2.896081
O	0.705380	-1.075163	1.827254
O	0.536955	1.369545	1.818151
H	-0.688958	2.230072	0.684787
O	1.003700	0.258038	3.902990
H	0.651672	-0.410287	4.519440
O	-1.193180	2.506124	-0.114227
H	-0.579759	2.294368	-0.854566
H	-2.558711	-0.581813	1.826690
O	-3.062937	-0.943478	1.055999
H	-3.009452	-0.029387	0.107175
H	-2.438647	-1.657693	0.704347
O	-1.137381	-2.491906	0.083577
H	-0.973830	-2.066945	-0.783455
H	-0.432366	-2.142650	0.669943
O	-2.885112	0.705783	-0.751495
H	-2.312754	0.230978	-1.420491
H	-2.271538	1.486771	-0.425068

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- A 0.00 kcal/mol

C	4.168445	-0.538498	-0.401832
N	2.720279	-0.267705	-0.270869
H	4.688687	-0.213224	0.502642
H	4.333347	-1.608969	-0.550427
H	4.560187	0.009650	-1.262845
H	0.186981	0.427069	-4.829940
H	2.191344	-0.530829	-1.138850
S	-0.007480	0.051947	-2.741599
O	1.252538	-0.690035	-2.569833
O	0.185647	1.003466	-4.043592
O	-1.156727	-0.809532	-3.042136
H	2.276774	-0.752850	0.541721
O	-0.250092	1.044516	-1.676613
H	2.492325	0.759308	-0.115029
S	0.249083	-0.451422	2.630423
O	-1.110105	-1.013657	2.608701
O	1.220561	-1.239983	1.861830
O	0.314700	0.997522	2.362585
H	-1.117316	2.051753	2.198815
O	0.713139	-0.519322	4.185213
H	0.504969	-1.413342	4.513324
O	-1.891258	2.576767	1.878998
H	-1.605400	3.501609	1.880092
H	-2.184912	-1.027350	1.377265
O	-2.843274	-0.973242	0.619213
H	-2.757749	0.074474	0.173433
H	-2.566272	-1.655469	-0.093629
O	-2.151944	-2.580827	-1.284344
H	-1.751224	-1.989971	-1.979389
H	-1.476785	-3.244635	-1.080649
O	-2.618795	1.275974	-0.312579
H	-2.368109	1.868664	0.460781

H	-1.829842	1.253135	-0.913001
O	1.630545	2.186906	0.155784
H	0.951821	2.018286	-0.533577
H	1.193436	1.900766	0.989321

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- B 1.35 kcal/mol

C	2.910244	1.892108	-0.217309
N	2.390821	0.556801	0.168984
H	3.905910	1.779408	-0.653782
H	2.236163	2.331393	-0.956431
H	2.968253	2.529374	0.668753
H	-0.660365	0.031828	4.759059
H	1.457171	0.636540	0.628463
S	-0.202067	-0.319264	2.703863
O	1.011966	-1.082736	2.994282
O	-0.495029	0.622244	4.001144
O	-0.030973	0.706126	1.648429
H	2.273004	-0.055341	-0.678075
O	-1.388790	-1.165494	2.529846
H	3.008494	0.081342	0.873928
S	0.677613	-0.460169	-2.727636
O	0.340270	0.919034	-2.309339
O	1.929381	-0.929503	-2.115903
O	-0.423492	-1.423021	-2.640306
H	-4.229770	-1.010818	1.250525
O	0.983302	-0.257367	-4.312651
H	1.080089	-1.144364	-4.705362
O	-3.410033	-0.677098	0.858054
H	-2.677777	-0.929587	1.490238
H	-1.148755	1.397136	-2.118143
O	-2.129071	1.578721	-1.897002
H	-2.170512	1.803804	-0.870237
H	-2.571239	0.600964	-1.950240
O	-2.325762	1.905227	0.613440
H	-1.479770	1.618026	1.037415
H	-2.929712	1.151474	0.809955
O	3.610641	-0.573621	2.379554
H	2.715262	-0.793744	2.742251
H	4.108233	-1.403698	2.400232
O	-2.978547	-0.777821	-1.893798
H	-2.122078	-1.207722	-2.141545
H	-3.119449	-0.952859	-0.931678

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- C 1.37 kcal/mol

C	3.730413	0.113248	1.860334
N	2.458869	0.260478	1.115694
H	3.994707	1.057519	2.344592
H	3.608944	-0.662259	2.620847
H	4.525866	-0.180321	1.170265
H	-1.580236	0.399756	4.575254
H	2.143979	-0.669221	0.668202
S	-0.702279	-0.305171	2.768451

O	0.069774	-1.526987	2.577037
O	-0.859495	-0.226963	4.381243
O	0.058471	0.920692	2.378281
H	1.660746	0.536037	1.738084
O	-2.068987	-0.295669	2.234446
H	2.508761	0.974593	0.363442
S	0.023735	-0.439353	-2.877723
O	-0.938110	0.616240	-3.245406
O	1.396891	0.071034	-2.703834
O	-0.424099	-1.314248	-1.784402
H	-2.071897	-1.144967	-0.798365
O	0.081055	-1.457242	-4.132472
H	0.341993	-0.947488	-4.921688
O	-2.804930	-0.675652	-0.341467
H	-2.559460	-0.655112	0.621642
H	-1.862468	1.308766	-2.101565
O	-2.370196	1.587088	-1.272568
H	-1.654401	2.021540	-0.637433
H	-2.635432	0.631475	-0.826606
O	-0.575868	2.567342	0.235828
H	-0.467344	2.023642	1.055775
H	0.288622	2.490356	-0.233713
O	1.456531	-2.056233	0.209913
H	0.847933	-2.126126	0.978724
H	0.869384	-1.903539	-0.564741
O	1.886944	2.055093	-1.041352
H	1.693306	1.360958	-1.744364
H	2.345296	2.777974	-1.493829

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- D 1.60 kcal/mol

C	3.643482	0.414743	1.616021
N	2.474511	0.438116	0.705868
H	3.859347	1.426160	1.971050
H	3.417632	-0.231787	2.468003
H	4.511551	0.021363	1.080383
H	-0.783080	-0.754699	4.781418
H	2.236309	-0.548065	0.368278
S	-0.401533	-0.360899	2.722010
O	0.585417	-1.428183	2.559729
O	-0.435384	0.020493	4.302912
O	0.039287	0.929423	2.128861
H	1.623898	0.766493	1.208672
O	-1.777034	-0.729963	2.367917
H	2.638672	1.040345	-0.140620
S	-0.128703	-0.300157	-2.827296
O	-0.966752	0.912826	-2.750932
O	1.290826	0.000348	-3.034652
O	-0.389017	-1.280498	-1.758279
H	-1.881544	-1.372579	-0.720814
O	-0.622459	-1.111767	-4.142165
H	-0.476897	-0.537537	-4.916465
O	-2.656534	-1.105878	-0.168217

H	-2.329049	-1.087441	0.770213
H	-2.081442	1.199446	-1.670664
O	-2.768695	1.246213	-0.920884
H	-2.377329	1.827338	-0.164790
H	-2.795728	0.211672	-0.548481
O	-1.741354	2.611538	1.003013
H	-1.111150	2.013330	1.492013
H	-2.372304	2.928648	1.665726
O	1.686793	-2.075380	0.022802
H	1.169631	-2.171110	0.849833
H	1.016954	-1.952522	-0.685907
O	2.679445	1.871708	-1.655629
H	2.158050	1.265896	-2.245537
H	3.481463	2.089622	-2.150751

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- E 1.65 kcal/mol

C	3.672180	1.515600	-0.188269
N	2.402582	0.755309	-0.223210
H	4.227271	1.331780	-1.111690
H	3.460159	2.584499	-0.100095
H	4.270541	1.190839	0.667060
H	0.672712	-1.615402	4.297444
H	1.840051	0.877516	0.645392
S	0.158231	-0.476579	2.570493
O	0.795121	0.778532	2.112269
O	1.052776	-0.820262	3.879689
O	-1.223593	-0.322840	3.023202
H	1.807326	1.013989	-1.049625
O	0.347038	-1.601604	1.633620
H	2.542876	-0.296049	-0.317038
S	-0.144520	0.092934	-2.811085
O	-1.513791	0.602122	-2.626112
O	0.887199	1.091807	-2.493162
O	0.099470	-1.231891	-2.214563
H	-1.048616	-2.035462	-1.044840
O	-0.000452	-0.221870	-4.395047
H	-0.226167	0.593241	-4.880064
O	-1.650111	-2.199334	-0.279061
H	-1.063578	-2.082201	0.503740
H	-2.547552	-1.027166	-0.419867
O	-3.061819	-0.133164	-0.643575
H	-2.530403	0.244644	-1.415896
H	-2.974912	0.513121	0.213305
O	-2.867041	1.250256	1.421395
H	-2.444719	0.649932	2.081320
H	-2.216176	2.003588	1.374246
O	2.276718	-1.951001	-0.477033
H	1.634889	-1.901219	-1.218220
H	1.706751	-2.060171	0.313527
O	-0.785753	2.990671	1.542176
H	-0.178567	2.285697	1.869960
H	-0.848505	3.634992	2.262500

$(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_5$ - F 1.69 kcal/mol

C	3.751700	0.282056	0.739672
N	2.317741	0.116429	0.408250
H	3.850686	0.645483	1.765794
H	4.250467	-0.685700	0.646058
H	4.208938	0.992825	0.046518
H	0.343796	0.522446	-4.566824
H	2.158539	-0.217993	-0.587943
S	0.471200	0.166169	-2.459549
O	1.683498	-0.603908	-2.114859
O	0.786487	0.984811	-3.782170
O	-0.685541	-0.709238	-2.788208
H	1.831508	-0.545613	1.071513
O	0.168516	1.177585	-1.428598
H	1.798322	0.997625	0.487487
S	0.079863	-0.439299	2.972127
O	-1.365698	-0.712513	2.989237
O	0.841596	-1.399232	2.146216
O	0.453903	0.956204	2.700554
H	-0.772866	2.191190	2.394674
O	0.575485	-0.641228	4.504795
H	0.194689	-1.477940	4.829245
O	-1.473049	2.793105	2.037571
H	-1.097419	3.684443	2.055335
H	-2.257452	-0.716957	1.604752
O	-2.738721	-0.659264	0.723615
H	-2.503682	0.377326	0.283288
H	-2.318797	-1.369028	0.113277
O	-1.626778	-2.369989	-0.873939
H	-1.229050	-1.827259	-1.607855
H	-0.882165	-2.833226	-0.460694
O	-2.206830	1.546316	-0.188166
H	-1.946861	2.117866	0.597574
H	-1.381805	1.451093	-0.738156
O	-0.600432	-0.442461	-5.527416
H	-0.948113	-0.829831	-4.692764
H	-1.349612	0.024484	-5.927359

 $(\text{H}_2\text{SO}_4)_2(\text{CH}_3\text{NH}_2)(\text{H}_2\text{O})_5$ - G 1.97 kcal/mol

C	-3.669052	-1.057377	-0.302228
N	-2.228419	-0.771999	-0.109518
H	-3.964376	-0.767978	-1.313946
H	-3.841108	-2.127760	-0.165137
H	-4.255276	-0.498205	0.431543
H	-1.560349	0.718496	4.603319
H	-1.897494	-0.998535	0.867875
S	-0.664870	0.312887	2.711975
O	-1.272105	-1.010118	2.442492
O	-1.681623	1.096574	3.713249
O	0.614282	0.225777	3.423786
H	-1.629966	-1.266917	-0.826850

O	-0.675651	1.182207	1.525602
H	-2.013080	0.224620	-0.238844
S	-0.163385	-0.496942	-2.805005
O	1.298923	-0.344825	-2.833109
O	-0.612951	-1.707318	-2.090757
O	-0.912707	0.703105	-2.401441
H	-0.198721	2.309067	-2.254735
O	-0.602999	-0.680348	-4.357728
H	0.002577	-1.330869	-4.758235
O	0.256898	3.142869	-1.976135
H	-0.428734	3.825116	-1.949948
H	2.247165	0.099536	-1.571472
O	2.794206	0.476438	-0.817437
H	2.187850	1.276000	-0.303761
H	3.084416	-0.281648	-0.180658
O	3.568537	-1.415620	0.713577
H	3.007387	-1.627575	1.525938
H	4.475299	-1.307357	1.033933
O	1.472695	2.258349	0.216849
H	1.003406	2.701880	-0.553378
H	0.750341	1.896632	0.791252
O	2.110832	-1.965158	2.834545
H	1.462823	-2.669839	2.686860
H	1.566454	-1.176985	3.096778

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- H 2.00 kcal/mol

C	3.790050	-1.363260	0.512377
N	2.464478	-0.707427	0.469113
H	4.269057	-1.153784	1.472550
H	3.670928	-2.443669	0.395022
H	4.414026	-0.977240	-0.297882
H	0.537055	0.450150	-4.440303
H	1.969764	-0.865108	-0.443749
S	0.241902	0.245067	-2.342271
O	1.167189	-0.835768	-1.965353
O	0.834028	0.968776	-3.628130
O	-1.092505	-0.275836	-2.750703
H	1.845454	-1.017721	1.253139
O	0.161124	1.316988	-1.333208
H	2.517396	0.347891	0.572768
S	-0.210095	-0.217401	3.043881
O	-1.567354	-0.773313	2.888741
O	0.844282	-1.172446	2.678574
O	-0.038748	1.128054	2.468727
H	-1.178566	1.833673	1.261785
O	-0.034398	0.074478	4.628971
H	-0.165375	-0.768474	5.101088
O	-1.781521	1.937741	0.483605
H	-1.184739	1.782476	-0.293530
H	-2.587039	0.817048	0.654563
O	-3.104883	-0.113176	0.903077
H	-2.562314	-0.469896	1.685095

H	-2.996426	-0.749562	0.093788
O	-2.772794	-1.595464	-1.152483
H	-2.113658	-1.135013	-1.749050
H	-3.571845	-1.718852	-1.685451
O	2.100924	1.992533	0.707435
H	1.464706	1.903774	1.448002
H	1.526058	2.024079	-0.086402
O	-0.394050	-0.535954	-5.452160
H	-0.947893	-0.722756	-4.662498
H	0.022505	-1.381034	-5.679504

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- I 2.20 kcal/mol

C	3.624848	-0.742708	1.971180
N	2.443355	-0.345028	1.174153
H	3.518384	-0.357381	2.988565
H	3.704175	-1.832771	2.001454
H	4.527186	-0.324442	1.517615
H	2.032389	-0.313165	-4.123172
H	2.483844	-0.665457	0.182589
S	1.055605	-0.142843	-2.234962
O	2.179179	-0.806355	-1.564760
O	1.622038	0.428942	-3.641543
O	-0.031208	-1.086874	-2.585648
H	1.546998	-0.704488	1.576347
O	0.575662	1.080539	-1.573902
H	2.318298	0.713842	1.109726
S	-0.777959	0.076843	2.743864
O	-2.176573	0.323584	2.350011
O	-0.166842	-1.047748	1.977399
O	0.083524	1.246044	2.824842
H	-2.350862	1.060585	-2.640412
O	-0.851407	-0.421879	4.285762
H	-1.591634	-1.051683	4.358791
O	-2.194408	1.511933	-1.763683
H	-1.210102	1.511747	-1.683943
H	-2.681533	0.645848	-0.785298
O	-3.029995	-0.100772	-0.072398
H	-2.761723	0.171403	0.865900
H	-2.443302	-0.953383	-0.241006
O	-1.435893	-2.063607	-0.331064
H	-0.857065	-1.854016	-1.101141
H	-0.903754	-1.858492	0.473434
O	1.778735	2.263173	0.811946
H	1.043588	2.210349	1.459434
H	1.361150	2.115434	-0.061357
O	-2.192734	-0.004006	-3.999218
H	-2.883963	-0.656118	-4.184243
H	-1.427600	-0.514161	-3.643802

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- J 3.31 kcal/mol

C	4.144048	-0.620363	0.164582
N	2.733598	-0.250957	-0.084663

H	4.277682	-1.695402	0.016743
H	4.789915	-0.075355	-0.528783
H	4.412664	-0.360369	1.191926
H	0.833657	0.043350	4.570228
H	2.529440	0.790904	0.029733
S	0.080653	-0.222496	2.590566
O	0.177290	1.217607	2.219451
O	1.167690	-0.431304	3.786910
O	-1.231463	-0.583813	3.096566
H	2.419250	-0.456585	-1.061110
O	0.630534	-1.119573	1.553764
H	2.066087	-0.717766	0.570009
S	0.189725	0.008543	-2.687455
O	-0.216221	1.111114	-1.779801
O	1.626266	-0.290435	-2.619962
O	-0.676148	-1.169475	-2.603533
H	-3.963036	-1.570730	-1.054376
O	-0.072300	0.678068	-4.141974
H	0.138126	0.007133	-4.817478
O	-3.451578	-1.172842	-0.334384
H	-2.608846	-1.750417	-0.225998
H	-1.711466	1.120600	-1.179811
O	-2.622651	1.140688	-0.731483
H	-2.987877	0.135660	-0.631578
H	-2.515056	1.512249	0.242649
O	-2.379122	1.958219	1.664462
H	-2.868430	1.338926	2.232452
H	-1.431848	1.789720	1.923242
O	-1.221215	-2.474993	-0.207594
H	-0.853325	-2.123162	-1.051003
H	-0.639334	-2.116178	0.496475
O	1.710244	2.247011	0.116441
H	1.087392	2.118194	-0.629182
H	1.168860	2.029173	0.910333

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- K 3.41 kcal/mol

C	4.067521	-0.069796	1.953073
N	2.796256	-0.245350	1.214961
H	3.904273	0.595947	2.804425
H	4.425559	-1.038172	2.313356
H	4.816608	0.370709	1.289391
H	1.134978	1.224410	-4.258238
H	2.906667	-0.878078	0.382965
S	0.046612	0.301221	-2.668545
O	0.441354	-0.890352	-1.890306
O	1.323777	0.472140	-3.667230
O	-1.142717	0.108344	-3.493613
H	2.039713	-0.607020	1.835935
O	-0.000220	1.543292	-1.864946
H	2.405772	0.683233	0.855879
S	-0.719732	-0.131743	2.643829
O	-1.620109	-1.123330	2.023265

O	0.615873	-0.674210	2.912306
O	-0.723174	1.187089	1.987879
H	-1.814275	1.708774	0.607867
O	-1.371003	0.221236	4.087894
H	-1.462349	-0.614108	4.582241
O	-2.308506	1.703621	-0.247069
H	-1.596950	1.748469	-0.930358
H	-2.846179	0.363950	-0.202419
O	-3.139682	-0.649701	-0.018711
H	-2.605993	-0.891632	0.815599
H	-2.777344	-1.235543	-0.806412
O	-2.179656	-2.013727	-1.949572
H	-2.191589	-1.411224	-2.725335
H	-1.216567	-2.027046	-1.760357
O	1.524852	2.021091	0.454929
H	0.774359	1.904201	1.078522
H	1.105981	1.898779	-0.428607
O	2.861651	-1.797359	-1.084496
H	2.010930	-1.489909	-1.490873
H	3.517895	-1.746245	-1.793944

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- L 3.81 kcal/mol

C	4.207055	0.306654	0.691194
N	2.743203	0.290319	0.480576
H	4.707703	0.101823	-0.258757
H	4.522055	1.287959	1.057496
H	4.486417	-0.461491	1.417385
H	-0.092294	-1.689795	4.436859
H	2.207422	0.458551	1.350303
S	-0.331279	-0.439716	2.729695
O	-0.291812	-1.600649	1.842649
O	0.360801	-0.882129	4.131534
O	0.563703	0.676076	2.326303
H	2.425783	1.038316	-0.209278
O	-1.689143	0.018148	3.058467
H	2.381656	-0.660192	0.127078
S	-0.298885	-0.433296	-2.959810
O	-1.446997	-0.526400	-2.007479
O	0.255012	0.912905	-3.050488
O	0.647253	-1.532227	-2.760146
H	-3.814035	-0.861860	0.936214
O	-0.936629	-0.653408	-4.435234
H	-1.116126	-1.606171	-4.534320
O	-3.593504	0.045321	1.197344
H	-2.919889	-0.043485	1.932816
H	-1.922781	0.576148	-1.281039
O	-2.360609	1.306781	-0.628011
H	-1.626179	1.807453	-0.144868
H	-2.899557	0.779248	0.100078
O	1.759392	2.225866	-1.173949
H	1.292688	1.784001	-1.926176
H	1.031075	2.581630	-0.626377

O	1.628084	-2.044748	-0.225677
H	0.882817	-2.045383	0.412341
H	1.221633	-1.958195	-1.122036
O	-0.435042	2.531149	0.712487
H	-0.711676	3.319438	1.203457
H	-0.102919	1.874554	1.397040

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- M 5.17 kcal/mol

C	-3.804667	0.072575	-0.517349
N	-2.502967	0.483729	0.059588
H	-4.215557	0.894904	-1.108460
H	-3.651827	-0.792348	-1.167382
H	-4.497672	-0.185724	0.287486
H	0.481814	-1.166649	4.595476
H	-2.068200	-0.270073	0.637392
S	-0.055973	-0.642189	2.597938
O	-0.204626	0.792288	2.899379
O	-0.235041	-1.443191	3.995442
O	-1.111245	-1.226159	1.773072
H	-1.803818	0.717477	-0.696882
O	1.317046	-0.954036	2.124307
H	-2.588004	1.299658	0.712500
S	-0.458856	0.069403	-2.966037
O	0.906441	0.050692	-3.532075
O	-0.575689	0.958533	-1.800396
O	-1.519763	0.120265	-3.947563
H	2.032087	2.021291	2.230261
O	-0.634053	-1.431786	-2.207821
H	-0.776484	-2.081720	-2.919997
O	2.733696	1.411663	1.952332
H	2.299887	0.526121	2.040841
H	2.095019	-0.065824	-2.567796
O	2.834236	-0.300587	-1.887445
H	2.375075	-0.987572	-1.226562
H	3.123512	0.544216	-1.351280
O	1.582479	-1.943339	-0.445363
H	0.702397	-1.893268	-0.876154
H	1.444535	-1.666777	0.494798
O	-2.430439	2.244978	2.200213
H	-1.637923	1.784245	2.574939
H	-2.216151	3.188556	2.212428
O	3.553574	1.720370	-0.528374
H	4.513585	1.840140	-0.490384
H	3.240837	1.638820	0.429693

(H₂SO₄)₂(CH₃NH₂)(H₂O)₅- N 5.97 kcal/mol

C	-1.557646	3.296154	-0.290660
N	-1.000467	1.924261	-0.307298
H	-2.119667	3.442929	0.635181
H	-0.750375	4.031766	-0.344644
H	-2.229506	3.424098	-1.143425
H	-0.294607	-1.270444	-4.938665

H	-0.472859	1.727518	-1.177532
S	-0.242586	-0.422750	-2.984038
O	-1.694559	-0.338288	-2.948387
O	0.201549	-0.530811	-4.541364
O	0.455231	0.819205	-2.569746
H	-0.349497	1.759860	0.492814
O	0.300226	-1.632120	-2.323155
H	-1.783825	1.167790	-0.260477
S	0.972392	0.186830	2.537800
O	0.821572	-1.040012	1.689924
O	0.786930	1.422387	1.781412
O	0.240533	0.067090	3.793031
H	-1.069240	-1.702023	1.486086
O	2.549382	0.252637	2.920759
H	2.703060	-0.398412	3.630206
O	-2.043081	-1.775851	1.466161
H	-2.300144	-1.588423	2.403773
H	1.584693	-1.219034	0.426976
O	2.051962	-1.411571	-0.487485
H	2.534503	-0.561099	-0.824734
H	1.320028	-1.565911	-1.202112
O	2.944547	0.727708	-1.558971
H	2.110387	0.860270	-2.086585
H	3.668181	0.653096	-2.198531
O	-2.856587	0.027132	-0.303575
H	-2.706161	-0.358284	-1.188727
H	-2.608600	-0.689527	0.361210
O	-2.286938	-1.101269	4.133762
H	-1.411773	-0.651698	4.128895
H	-2.918494	-0.424410	4.416219

(H₂SO₄)₂(CH₃NH₂)₂- A 0.00 kcal/mol

C	3.428078	-0.632587	0.329441
N	2.072957	-0.155736	-0.031803
H	3.444536	-1.723180	0.263418
H	4.164498	-0.216849	-0.363300
H	3.661791	-0.328200	1.352821
H	1.341482	-0.520062	0.643895
H	1.995337	0.864056	0.022207
S	-0.025747	0.063697	-2.699274
O	-0.238895	0.965311	-1.540595
O	-1.192979	-0.706312	-3.101470
O	0.277619	1.138474	-3.890602
H	0.241325	0.646006	-4.730705
O	1.213671	-0.730101	-2.538977
H	1.790749	-0.428308	-1.019916
C	-2.701921	-1.142960	-0.136355
N	-2.347276	0.293394	0.034783
H	-3.590917	-1.371547	0.457099
H	-2.870371	-1.350439	-1.195431
H	-1.860017	-1.736061	0.227619
H	-1.546357	0.560756	-0.608780

H	-3.138005	0.902150	-0.186896
S	-0.166890	0.046526	2.784972
O	0.168762	-0.934758	1.728972
O	0.093954	-0.349605	4.150323
O	0.934107	1.245724	2.427300
H	0.957599	1.837722	3.200027
O	-1.495347	0.659525	2.558691
H	-2.033300	0.484010	1.038268

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)- A 0.00 kcal/mol

C	3.408448	-1.408139	0.179195
N	2.135799	-0.701287	-0.082802
H	3.251937	-2.487802	0.108051
H	4.156077	-1.100555	-0.556640
H	3.761659	-1.160051	1.183696
H	1.399823	-0.929204	0.626962
H	2.225834	0.352766	-0.040395
S	-0.200122	-0.009652	-2.705538
O	-0.318990	0.934397	-1.558722
O	-1.450307	-0.677143	-3.033868
O	0.146975	1.025832	-3.916005
H	0.213642	0.500056	-4.734027
O	0.966466	-0.902452	-2.583032
H	1.741823	-0.901897	-1.036336
C	-2.857364	-1.153098	-0.105704
N	-2.461616	0.275561	0.039229
H	-3.735548	-1.349090	0.514833
H	-3.059349	-1.367024	-1.157210
H	-2.021862	-1.763512	0.243786
H	-1.660999	0.515500	-0.608056
H	-3.237497	0.901596	-0.187462
S	-0.302267	-0.035838	2.802267
O	0.039488	-0.964284	1.709209
O	-0.124066	-0.513043	4.155367
O	0.867006	1.149077	2.599707
H	0.958118	1.585974	3.465251
O	-1.586315	0.655629	2.546861
H	-2.135868	0.471798	1.038868
O	1.799833	2.027271	-0.015564
H	1.379749	2.022384	0.867198
H	1.054193	1.902140	-0.643738

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)- B 0.28 kcal/mol

C	-3.559739	0.644469	0.009373
N	-2.345946	-0.191992	0.156722
H	-3.825930	1.074906	0.978099
H	-3.346441	1.444065	-0.704258
H	-4.385428	0.033416	-0.364033
H	-2.460450	-0.936256	0.859783
H	-2.034711	-0.596253	-0.771346
S	-0.250197	-0.137282	2.755640
O	-1.394904	-1.047396	2.702679

O	0.090800	0.418336	4.046809
O	1.083030	-1.086238	2.328166
H	1.368993	-1.532050	3.144816
O	-0.247759	0.820780	1.616496
H	-1.539942	0.357739	0.552879
C	3.923956	-0.300251	-0.126621
N	2.456839	-0.124826	-0.038414
H	4.403600	0.176494	0.732539
H	4.171914	-1.365138	-0.140661
H	4.285243	0.165411	-1.047018
H	1.957997	-0.540963	-0.867229
H	2.060465	-0.540707	0.824850
S	-0.201735	-0.259291	-2.562971
O	-1.419660	-1.042851	-2.263794
O	1.053479	-0.948746	-2.245479
O	-0.121914	-0.165940	-4.183095
H	-0.966029	0.205826	-4.497318
O	-0.297893	1.118085	-2.049931
H	0.783923	2.098251	-0.907963
O	1.360239	2.354352	-0.149994
H	2.162749	0.903782	-0.043428
H	0.790082	2.186021	0.628048

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)- C 0.31 kcal/mol

C	3.433133	0.587506	-1.137027
N	2.126037	0.129015	-0.611938
H	3.459593	1.679416	-1.104580
H	4.241961	0.187273	-0.520194
H	3.548884	0.253263	-2.171209
H	1.325837	0.480704	-1.211976
H	2.042020	-0.891364	-0.627356
S	0.391342	0.001190	2.332427
O	-0.020384	-0.895129	1.218468
O	-0.731559	0.797355	2.860752
O	0.890284	-0.952403	3.511251
H	0.220606	-0.904480	4.263277
O	1.575347	0.793885	1.950517
H	1.956056	0.433973	0.393396
C	-2.538352	1.250452	0.015255
N	-2.248938	-0.201255	-0.143921
H	-3.490909	1.487983	-0.465202
H	-2.561186	1.500358	1.078494
H	-1.735335	1.802536	-0.478199
H	-1.381341	-0.471830	0.410321
H	-3.022969	-0.775956	0.196057
S	-0.423863	-0.092208	-3.147994
O	0.053232	0.908994	-2.167553
O	-0.331959	0.268976	-4.544323
O	0.699248	-1.298071	-2.899815
H	0.605819	-1.919320	-3.643663
O	-1.720240	-0.679929	-2.741924
H	-2.069024	-0.435530	-1.169895

O	-1.058928	-0.421646	5.257050
H	-0.758451	0.087694	6.024471
H	-1.209933	0.243238	4.541592

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)- D 0.71 kcal/mol

C	3.524002	0.515402	-1.098904
N	2.212393	0.197938	-0.487765
H	3.621181	1.600692	-1.180611
H	4.331234	0.122893	-0.474953
H	3.572769	0.072892	-2.096949
H	1.405724	0.536653	-1.099171
H	2.057662	-0.811202	-0.392720
S	0.623987	-0.045584	2.484010
O	0.270687	-0.916055	1.346915
O	-0.528331	0.512946	3.200830
O	1.341432	-1.103311	3.497721
H	1.582364	-0.611753	4.304346
O	1.647970	0.957568	2.134406
H	2.098435	0.593441	0.480707
C	-2.170306	1.614276	0.194172
N	-2.057834	0.131627	0.138176
H	-3.180249	1.907120	-0.103165
H	-1.970903	1.948612	1.215123
H	-1.441813	2.039939	-0.499013
H	-1.128431	-0.190304	0.492060
H	-2.737020	-0.303017	0.791754
S	-0.422510	-0.124209	-2.925703
O	0.145837	0.917974	-2.033081
O	-0.260172	0.095745	-4.345484
O	0.578201	-1.399558	-2.530369
H	0.414196	-2.094966	-3.191857
O	-1.773927	-0.537349	-2.502853
H	-2.127899	-0.209757	-0.856226
O	-3.097176	-0.463485	2.660953
H	-3.311431	-1.288413	3.118579
H	-2.209691	-0.196968	3.002413

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)- E 2.45 kcal/mol

C	2.779944	0.313222	2.878892
N	2.165443	0.226283	1.530093
H	2.051779	-0.043190	3.612199
H	3.686116	-0.297645	2.911391
H	3.034849	1.355893	3.084990
H	1.236039	0.734588	1.497496
H	2.784113	0.590968	0.760222
S	-0.959489	-0.377184	2.044469
O	-0.434913	-0.556634	3.384116
O	-2.383741	-0.541055	1.808547
O	-0.466195	0.931096	1.428685
H	-1.434725	1.400818	0.235689
O	-0.167315	-1.518671	1.187409
H	1.883060	-0.738898	1.303832

C	-3.305427	1.063593	-0.740668
N	-1.975971	1.723873	-0.636693
H	-3.880523	1.258694	0.166585
H	-3.831825	1.439568	-1.622637
H	-3.138142	-0.011085	-0.827251
H	-1.359681	1.476948	-1.460926
H	-2.065128	2.741335	-0.590867
S	0.247602	-0.403278	-2.252880
O	1.614489	-0.427449	-1.731866
O	-0.253803	0.939259	-2.617394
O	0.405239	-1.220927	-3.647146
H	-0.478215	-1.289035	-4.052647
O	-0.728003	-1.149922	-1.435747
H	-0.423886	-1.442166	0.222266
O	3.421175	1.243816	-0.706916
H	4.303803	1.068079	-1.062573
H	2.793687	0.734430	-1.283840

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)- F 2.69 kcal/mol

C	-3.382475	1.592483	-1.443094
N	-2.288367	0.706248	-0.988803
H	-3.302291	1.738293	-2.523341
H	-4.348007	1.140382	-1.201445
H	-3.297923	2.555934	-0.934332
H	-1.319766	1.061112	-1.230562
H	-2.271281	0.538731	0.053445
S	0.361237	-0.344618	-2.411807
O	-0.527542	-0.223885	-3.551233
O	1.717249	-0.823543	-2.627219
O	0.368728	0.920243	-1.562341
H	1.725793	0.886392	-0.626675
O	-0.417558	-1.422681	-1.458160
H	-2.307390	-0.217835	-1.441850
C	3.295743	-0.379198	0.074761
N	2.632303	0.949646	-0.061414
H	3.443502	-0.803669	-0.919983
H	4.244669	-0.256200	0.603802
H	2.629208	-1.024165	0.650834
H	2.411598	1.345127	0.895513
H	3.238344	1.605836	-0.559299
S	-0.742197	-0.422415	2.177574
O	-1.966151	0.204056	1.665430
O	-0.060454	0.334494	3.237913
O	-1.334460	-1.756206	2.893980
H	-0.608500	-2.160599	3.402971
O	0.192942	-0.879878	1.128987
H	-0.127136	-1.306626	-0.508930
O	2.125617	1.708604	2.520766
H	1.319941	1.198541	2.820903
H	1.990477	2.610681	2.843208

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₂- A 0.00 kcal/mol

C	-3.159678	1.363816	-0.141909
N	-2.302369	0.180634	0.111083
H	-3.344493	1.887097	0.799699
H	-2.646936	2.026410	-0.843679
H	-4.110373	1.039046	-0.572614
H	-2.738711	-0.484000	0.796676
H	-2.071105	-0.310484	-0.791055
S	0.399648	0.130816	2.721877
O	-0.755099	-0.405723	3.449328
O	1.429731	0.746910	3.528299
O	1.126925	-1.228690	2.023652
H	1.501732	-1.741772	2.762156
O	0.034423	0.867082	1.488933
H	-1.398762	0.466819	0.557497
C	3.948304	-0.652157	-0.576343
N	2.505540	-0.362005	-0.416417
H	4.504545	-0.218941	0.259352
H	4.110988	-1.733083	-0.605197
H	4.299642	-0.210607	-1.512362
H	1.930166	-0.734118	-1.217669
H	2.120540	-0.750088	0.464104
S	-0.320608	-0.275668	-2.736004
O	-1.573162	-0.931235	-2.310147
O	0.891229	-1.071507	-2.506833
O	-0.372623	-0.225557	-4.360260
H	-1.219681	0.184022	-4.613197
O	-0.239413	1.116965	-2.260333
H	0.974681	1.990120	-1.191318
O	1.623962	2.198562	-0.478306
H	2.295937	0.688602	-0.406986
H	1.098962	2.096923	0.342167
O	-3.079326	-1.269825	2.326554
H	-3.168896	-2.228392	2.422260
H	-2.250007	-1.026154	2.815958

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₂- B 0.02 kcal/mol

C	3.867370	0.138570	0.951392
N	2.425353	-0.022443	0.655936
H	4.316702	0.816783	0.221464
H	3.993449	0.540605	1.959987
H	4.354163	-0.837576	0.885299
H	2.253603	-0.382172	-0.328951
H	1.939781	-0.640508	1.360271
S	0.718199	0.207358	-2.281247
O	1.854182	-0.665154	-1.918689
O	0.738985	0.665338	-3.670899
O	-0.619320	-0.750797	-2.161705
H	-0.843622	-1.067512	-3.094521
O	0.480982	1.243581	-1.267205
H	1.916142	0.868864	0.704446
C	-3.840259	-0.195881	-0.316230
N	-2.397071	-0.001047	-0.051638

H	-4.122520	0.346256	-1.222756
H	-4.054359	-1.260169	-0.446870
H	-4.416320	0.187745	0.529728
H	-2.087147	-0.479882	0.830927
H	-1.805184	-0.337102	-0.839092
S	-0.186803	-0.373148	2.807619
O	0.928756	-1.307551	2.557044
O	-1.492087	-0.915299	2.388434
O	-0.280667	-0.193793	4.421515
H	-0.517561	-1.061148	4.797885
O	0.091971	0.993042	2.349462
H	-0.915414	2.160665	1.241871
O	-1.385060	2.474417	0.436583
H	-2.139423	1.025181	0.097279
H	-0.710277	2.362180	-0.266272
O	-0.968904	-1.140115	-4.757878
H	-0.518592	-1.896255	-5.163317
H	-0.297106	-0.414361	-4.743693

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₂- C 0.02 kcal/mol

C	3.866245	0.135174	0.952466
N	2.424036	-0.025829	0.657825
H	4.314995	0.813504	0.222294
H	3.992721	0.537199	1.961014
H	4.353170	-0.840895	0.886083
H	2.251308	-0.383881	-0.327520
H	1.939114	-0.644904	1.361366
S	0.719527	0.206723	-2.281217
O	1.856529	-0.664509	-1.918579
O	0.740523	0.665900	-3.670552
O	-0.616561	-0.753335	-2.163526
H	-0.843556	-1.064782	-3.097641
O	0.480802	1.241982	-1.266458
H	1.914451	0.865113	0.709342
C	-3.839420	-0.202234	-0.316814
N	-2.396151	-0.006588	-0.053609
H	-4.122393	0.337635	-1.224483
H	-4.053617	-1.266858	-0.444633
H	-4.414961	0.183485	0.528557
H	-2.086051	-0.482104	0.830779
H	-1.804419	-0.345268	-0.840104
S	-0.187010	-0.370512	2.808821
O	0.927295	-1.307400	2.562110
O	-1.492946	-0.911783	2.390382
O	-0.281743	-0.185718	4.422025
H	-0.520347	-1.051407	4.801145
O	0.094094	0.993911	2.346378
H	-0.919036	2.158668	1.239230
O	-1.389124	2.470668	0.433471
H	-2.138500	1.020336	0.091902
H	-0.713634	2.359681	-0.268965
O	-0.969847	-1.131279	-4.760328

H	-0.521245	-1.886556	-5.169252
H	-0.296614	-0.406556	-4.743593
(H ₂ SO ₄) ₂ (CH ₃ NH ₂) ₂ (H ₂ O) ₂ - D 0.61 kcal/mol			
C	-4.082549	-0.969382	0.479205
N	-2.689364	-0.497271	0.323628
H	-4.512577	-0.536333	1.386249
H	-4.673962	-0.660773	-0.386998
H	-4.097518	-2.059780	0.559177
H	-2.087251	-0.750235	1.149172
H	-2.236229	-0.849315	-0.548707
S	0.101840	-0.041163	2.707337
O	-1.104257	-0.869527	2.541280
O	0.443212	0.292281	4.072905
O	1.365835	-1.044612	2.194234
H	1.640428	-1.535842	2.988231
O	0.186834	1.043579	1.712519
H	-2.606776	0.559387	0.242652
C	4.105206	-0.928041	-0.513261
N	2.703669	-0.502570	-0.302390
H	4.726761	-0.576060	0.314618
H	4.159931	-2.018565	-0.573969
H	4.472999	-0.497784	-1.448365
H	2.074708	-0.791214	-1.097462
H	2.302961	-0.863976	0.582768
S	-0.214476	-0.170733	-2.514627
O	-1.399211	-0.940274	-2.107330
O	1.035420	-0.948604	-2.420033
O	-0.413322	0.158769	-4.094182
H	-0.519813	-0.691164	-4.559031
O	-0.126396	1.176450	-1.932101
H	1.321139	2.002928	-0.901576
O	1.981846	2.093430	-0.180881
H	2.587994	0.561040	-0.250801
H	1.441650	1.961318	0.629614
O	-1.938058	2.109342	0.071164
H	-1.264942	1.996910	0.775280
H	-1.418617	1.956568	-0.749134
(H ₂ SO ₄) ₂ (CH ₃ NH ₂) ₂ (H ₂ O) ₂ - E 2.10 kcal/mol			
C	3.813011	0.093002	0.208190
N	2.351933	0.065129	-0.034598
H	4.204800	-0.927383	0.206896
H	4.305869	0.677258	-0.572893
H	4.002881	0.548046	1.183900
H	1.864255	-0.417872	0.760885
H	1.939190	1.037913	-0.103278
S	0.019250	-0.452832	-2.830871
O	-0.431300	0.854551	-2.272936
O	-0.910067	-1.536978	-2.545094
O	-0.051523	-0.141964	-4.428883
H	0.197422	-0.962957	-4.891409

O	1.431672	-0.745763	-2.537339
H	2.098082	-0.393349	-0.941471
C	-3.476202	-0.338072	-0.642328
N	-2.209795	0.317954	-0.233543
H	-4.074278	-0.559658	0.245240
H	-4.031711	0.321514	-1.313939
H	-3.223674	-1.261917	-1.167649
H	-1.571468	0.473699	-1.059314
H	-2.341912	1.234759	0.219879
S	-0.041403	-0.784806	2.859126
O	1.294213	-0.948505	2.273112
O	-0.244938	-1.387221	4.158715
O	-0.111887	0.891194	3.186467
H	-0.244773	0.944395	4.148616
O	-1.127756	-0.968121	1.884616
H	-1.700081	-0.258718	0.486992
O	1.029205	2.436985	-0.510540
H	0.303825	2.605498	0.129073
H	0.572174	2.038342	-1.287916
O	-1.210295	2.552888	1.319601
H	-0.855156	2.017657	2.077823
H	-1.445405	3.417298	1.686539

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₂- F 2.74 kcal/mol

C	-3.715517	0.738112	-0.063105
N	-2.301483	0.312432	0.048995
H	-3.994076	1.309062	0.826293
H	-3.846973	1.355485	-0.955777
H	-4.350482	-0.148637	-0.133875
H	-2.124655	-0.262614	0.932893
H	-1.967581	-0.212615	-0.795215
S	-0.575478	-0.314549	2.951693
O	-1.765952	-0.962490	2.354231
O	-0.546862	-0.305773	4.397119
O	0.708289	-1.320272	2.503393
H	0.726662	-2.038825	3.159605
O	-0.219047	0.924013	2.249381
H	-1.657112	1.112443	0.104122
C	4.021186	-0.531501	0.619596
N	2.571394	-0.240185	0.556461
H	4.415306	-0.234784	1.595420
H	4.195420	-1.599561	0.462660
H	4.532424	0.034294	-0.163607
H	2.160501	-0.473420	-0.387871
H	2.027932	-0.745440	1.278979
S	0.225460	0.175332	-2.200593
O	-0.982793	-0.704578	-2.177583
O	1.458986	-0.575042	-1.908857
O	0.344692	0.713867	-3.697140
H	0.038133	-0.025702	-4.307222
O	0.048624	1.378943	-1.374939
H	1.171729	2.232413	-0.075959

O	1.685724	2.312945	0.758129
H	2.354114	0.799261	0.691091
H	1.025678	2.069885	1.444341
O	-0.756776	-1.445781	-4.848164
H	-1.086078	-1.530384	-3.924560
H	-1.543125	-1.285451	-5.390619

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₃- A 0.00 kcal/mol

C	3.986956	-0.419823	-0.120543
N	2.523022	-0.198838	-0.080077
H	4.420577	0.171318	-0.931230
H	4.426690	-0.112831	0.831929
H	4.194788	-1.478850	-0.294854
H	2.072850	-0.472457	-0.989157
H	2.079015	-0.725383	0.706137
S	0.123070	-0.393937	-2.924547
O	1.476922	-0.840557	-2.557449
O	-0.003653	0.187682	-4.243405
O	-0.826390	-1.739938	-2.888127
H	-0.631738	-2.243952	-3.698658
O	-0.520862	0.378095	-1.822936
H	2.282314	0.815855	0.126421
C	-3.702046	-1.012693	-0.324681
N	-2.420994	-0.378759	0.057067
H	-4.179765	-0.425673	-1.113594
H	-3.514844	-2.025073	-0.691879
H	-4.359925	-1.054721	0.547317
H	-1.934479	-0.888636	0.836070
H	-1.757440	-0.303572	-0.745448
S	0.068483	-0.592927	2.705496
O	1.348233	-1.159125	2.252983
O	-1.099561	-1.374354	2.261613
O	0.080491	-0.686842	4.327740
H	0.166768	-1.628243	4.565159
O	-0.062428	0.857177	2.484542
H	-1.573315	1.838165	1.776227
O	-2.230968	2.138881	1.111288
H	-2.529617	0.614616	0.420245
H	-1.688366	2.597077	0.430832
O	1.724045	2.276217	0.770009
H	1.185116	1.912420	1.507494
H	1.057450	2.658031	0.154938
O	-0.421101	2.904939	-0.951094
H	-0.487318	3.602580	-1.618897
H	-0.435097	2.040025	-1.443151

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₃- B 0.13 kcal/mol

C	3.995600	-0.397257	-0.119099
N	2.529404	-0.202477	-0.042445
H	4.395293	0.188738	-0.950645
H	4.455522	-0.066960	0.815902
H	4.218669	-1.454825	-0.282939

H	2.063140	-0.490100	-0.939669
H	2.114795	-0.725140	0.760994
S	0.139078	-0.391934	-2.931250
O	1.474237	-0.845537	-2.506767
O	0.067735	0.157438	-4.267587
O	-0.826377	-1.726320	-2.893415
H	-0.590998	-2.268466	-3.667756
O	-0.536451	0.413297	-1.873798
H	2.273470	0.809917	0.159565
C	-3.698292	-1.018983	-0.359055
N	-2.421366	-0.370301	0.011729
H	-4.199162	-0.426919	-1.129615
H	-3.500210	-2.021701	-0.746366
H	-4.339968	-1.087032	0.523277
H	-1.915017	-0.883140	0.775167
H	-1.768990	-0.276375	-0.798098
S	0.060487	-0.607441	2.712235
O	1.407773	-1.080591	2.360446
O	-1.038063	-1.400938	2.156251
O	-0.109271	-0.874960	4.305198
H	0.645372	-0.453280	4.755248
O	-0.095326	0.854171	2.517242
H	-1.580273	1.816676	1.772866
O	-2.235005	2.130308	1.109959
H	-2.537575	0.615462	0.390556
H	-1.690220	2.596202	0.437011
O	1.683658	2.254872	0.801734
H	1.034122	2.645739	0.174006
H	1.124475	1.875789	1.517996
O	-0.420637	2.918910	-0.949018
H	-0.479033	3.631837	-1.601128
H	-0.434752	2.065257	-1.460165

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₃- C 0.36 kcal/mol

C	4.052920	-0.411581	-0.186259
N	2.592074	-0.179347	-0.112470
H	4.479820	0.216360	-0.972704
H	4.512180	-0.157939	0.772710
H	4.248204	-1.461823	-0.418968
H	2.125670	-0.412402	-1.025615
H	2.147360	-0.731545	0.654476
S	0.093039	-0.386119	-2.885963
O	1.497115	-0.712514	-2.587808
O	-0.160569	0.089389	-4.228787
O	-0.753266	-1.788617	-2.697464
H	-0.595134	-2.321298	-3.497467
O	-0.533771	0.411741	-1.793811
H	2.359723	0.827843	0.137985
C	-3.770742	-0.947557	-0.337205
N	-2.480825	-0.333680	0.047473
H	-4.248277	-0.342037	-1.112219
H	-3.595922	-1.955128	-0.723363

H	-4.423928	-0.998934	0.537893
H	-1.992488	-0.862111	0.812993
H	-1.818209	-0.255117	-0.755391
S	0.068655	-0.624031	2.642420
O	1.341872	-1.185805	2.168153
O	-1.107231	-1.389207	2.191817
O	0.092808	-0.754341	4.262795
H	0.175005	-1.701348	4.477964
O	-0.057358	0.831580	2.457062
H	-1.586120	1.834596	1.803953
O	-2.241608	2.161443	1.149341
H	-2.574270	0.655087	0.425836
H	-1.687968	2.620822	0.478574
O	1.785612	2.258767	0.827366
H	1.120544	2.653046	0.218945
H	1.237679	1.870579	1.546434
O	-0.376394	2.920153	-0.869658
H	-0.436490	3.626705	-1.528595
H	-0.403971	2.062347	-1.373048

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₃- D 2.61 kcal/mol

C	-3.365509	1.276345	0.858592
N	-2.332141	0.230632	1.040601
H	-3.300108	1.992903	1.681189
H	-3.189190	1.783855	-0.093273
H	-4.358409	0.818415	0.853557
H	-2.411410	-0.248381	1.968961
H	-2.328719	-0.436850	0.242234
S	0.982430	0.003200	2.088556
O	0.665823	0.177499	3.502997
O	2.410339	-0.048755	1.736291
O	0.340787	-1.427466	1.741993
H	0.732453	-1.826182	0.896530
O	0.262468	0.985644	1.213945
H	-1.354037	0.639415	1.056382
C	3.865244	0.456992	-1.662691
N	2.546141	0.535490	-0.996078
H	4.560155	1.144934	-1.174661
H	4.251879	-0.563037	-1.589398
H	3.758950	0.731700	-2.715569
H	1.841554	-0.068023	-1.462697
H	2.588874	0.262645	0.021231
S	-1.047023	-0.278663	-2.273054
O	-1.972740	-1.068929	-1.448389
O	0.336450	-0.807833	-2.277016
O	-1.468274	-0.540320	-3.823191
H	-2.363590	-0.176285	-3.948037
O	-1.139391	1.167205	-2.045404
H	0.214355	2.365537	-1.414270
O	0.943238	2.737973	-0.870070
H	2.102625	1.502161	-1.025435
H	0.705829	2.421444	0.028880

O	-2.053094	-0.442348	3.739122
H	-2.102723	-1.333356	4.114523
H	-1.087688	-0.215394	3.775206
O	1.240011	-2.553631	-0.472392
H	0.764401	-2.096500	-1.214320
H	0.986955	-3.486797	-0.519227

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- A 0.00 kcal/mol

C	4.094962	-0.627932	0.484078
N	2.655689	-0.281203	0.485934
H	4.640430	0.097373	-0.125561
H	4.478968	-0.604825	1.507334
H	4.234191	-1.627473	0.063507
H	2.262117	-0.287179	-0.489730
H	2.093372	-0.925393	1.084580
S	0.390120	0.113110	-2.539612
O	1.760824	-0.206171	-2.113927
O	0.297097	0.640947	-3.902353
O	-0.452640	-1.260890	-2.502130
H	-0.558767	-1.577792	-3.454353
O	-0.326062	0.937388	-1.524601
H	2.473474	0.680333	0.906278
C	-3.762254	-0.388209	-0.595020
N	-2.475669	0.033370	0.001134
H	-4.125045	0.389590	-1.272356
H	-3.618188	-1.316046	-1.154666
H	-4.495937	-0.549727	0.199234
H	-2.103145	-0.665121	0.690339
H	-1.735768	0.197758	-0.717220
S	-0.263886	-0.950338	2.758900
O	1.012260	-1.559548	2.358258
O	-1.425247	-1.504699	2.043315
O	-0.475916	-1.337340	4.324453
H	-0.493394	-2.310010	4.383343
O	-0.241607	0.521835	2.811572
H	-1.585796	1.759007	2.195846
O	-2.125644	2.267764	1.551377
H	-2.532044	0.941925	0.547796
H	-1.451449	2.762234	1.033552
O	1.916596	2.019138	1.753689
H	1.246867	1.565330	2.314054
H	1.369188	2.556223	1.135942
O	0.071392	3.134640	-0.060722
H	0.160030	3.953245	-0.569556
H	0.010768	2.395082	-0.725575
O	-0.668813	-1.582240	-5.133451
H	0.011729	-2.103920	-5.584457
H	-0.295661	-0.669874	-5.064593

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- B 0.45 kcal/mol

C	-3.440620	-1.793703	-0.089452
N	-2.204743	-0.979567	-0.029989

H	-4.170770	-1.401184	0.623136
H	-3.854199	-1.746052	-1.099986
H	-3.209533	-2.832323	0.161235
H	-1.778608	-0.995361	0.923949
H	-1.507575	-1.304706	-0.736641
S	0.309090	-0.904127	2.614482
O	0.856988	-1.504058	1.393360
O	-1.163366	-0.775302	2.590734
O	0.659736	-2.032002	3.733420
H	0.420069	-1.666167	4.604318
O	0.982750	0.333139	3.046856
H	-2.382687	0.037738	-0.297303
C	3.903535	0.080427	0.128018
N	2.473111	0.042638	-0.249876
H	3.998045	0.493498	1.135746
H	4.316398	-0.931753	0.111269
H	4.450271	0.710599	-0.578331
H	2.314687	-0.343872	-1.208688
H	1.912218	-0.537837	0.418127
S	0.173199	-0.459619	-2.956120
O	-0.623048	-1.471502	-2.262193
O	1.630471	-0.620477	-2.834479
O	-0.183795	-0.756134	-4.513623
H	0.379344	-0.175364	-5.057188
O	-0.260946	0.935100	-2.694295
H	0.773453	2.029680	-1.570562
O	1.259991	2.412504	-0.805381
H	2.041133	1.013819	-0.290952
H	0.552210	2.785117	-0.228000
O	-2.420214	1.560032	-0.981911
H	-1.768466	1.414581	-1.706408
H	-1.995919	2.235857	-0.401292
O	-0.907487	2.302920	3.113450
H	-1.667100	1.709215	3.226756
H	-0.142844	1.668870	3.137488
O	-0.953697	3.280439	0.673919
H	-1.123897	4.232244	0.718819
H	-0.947993	2.944248	1.629529

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- C 1.04 kcal/mol

C	-3.423190	1.280961	0.487677
N	-2.112868	0.781086	0.009784
H	-3.333979	1.544414	1.544738
H	-3.709102	2.162495	-0.091979
H	-4.180275	0.501612	0.366091
H	-1.796621	-0.034958	0.583922
H	-2.132100	0.494910	-0.995944
S	-0.506544	-0.555559	2.859026
O	-1.160024	-1.239773	1.726604
O	-1.174683	0.662413	3.294280
O	-0.518543	-1.609341	4.101902
H	-1.446423	-1.712618	4.381408

O	0.959360	-0.409242	2.640639
H	-1.365817	1.531956	0.088923
C	2.637400	-2.562607	0.051080
N	1.825805	-1.323464	0.085507
H	3.439650	-2.493443	0.790280
H	2.001321	-3.421674	0.279255
H	3.068304	-2.683845	-0.946004
H	1.047519	-1.362859	-0.616438
H	1.410619	-1.163300	1.028884
S	-0.576887	-0.595005	-2.904733
O	-1.797658	0.205552	-2.715785
O	-0.238146	-1.431904	-1.748212
O	-0.920623	-1.708279	-4.039154
H	-1.164384	-1.229324	-4.852134
O	0.552536	0.184444	-3.447498
H	2.745250	1.520495	-0.993193
O	3.198711	1.032588	-0.264877
H	2.409224	-0.457702	-0.119335
H	2.917834	1.502064	0.552608
O	-0.156932	2.711235	0.094434
H	0.485036	2.584106	0.830301
H	0.388138	2.658121	-0.724592
O	1.834892	2.046256	1.990613
H	2.051664	2.616615	2.741895
H	1.492369	1.193041	2.377454
O	1.524488	2.264627	-2.128458
H	1.135640	1.517113	-2.674193
H	1.768191	2.959720	-2.756120

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- D 1.06 kcal/mol

C	4.073806	-0.655962	0.528806
N	2.637387	-0.297704	0.508674
H	4.632400	0.055213	-0.085493
H	4.445504	-0.619981	1.556207
H	4.209304	-1.663180	0.125775
H	2.254814	-0.315481	-0.470889
H	2.065070	-0.929696	1.111575
S	0.413402	0.091496	-2.546027
O	1.772246	-0.253731	-2.104179
O	0.346795	0.633733	-3.904681
O	-0.450224	-1.269707	-2.532394
H	-0.577167	-1.559851	-3.490861
O	-0.302503	0.919375	-1.533100
H	2.459648	0.670850	0.914092
C	-3.738903	-0.391330	-0.617657
N	-2.457180	0.028417	-0.009752
H	-4.088042	0.381938	-1.307204
H	-3.593498	-1.325440	-1.166391
H	-4.483399	-0.540358	0.168901
H	-2.097785	-0.665360	0.690900
H	-1.708916	0.183086	-0.721732
S	-0.281893	-0.933768	2.780422

O	0.991023	-1.555447	2.387951
O	-1.445467	-1.488327	2.068598
O	-0.498828	-1.303112	4.349476
H	-0.524099	-2.275003	4.418095
O	-0.249807	0.538599	2.817120
H	-1.584877	1.776772	2.176518
O	-2.116856	2.278064	1.519938
H	-2.515257	0.942479	0.527564
H	-1.437373	2.765653	1.002380
O	1.913204	2.024291	1.746913
H	1.239890	1.579692	2.310060
H	1.371202	2.558562	1.122044
O	0.085988	3.130427	-0.090290
H	0.178660	3.944317	-0.605901
H	0.028788	2.384676	-0.748603
O	-0.707544	-1.529769	-5.164940
H	-0.051949	-2.066735	-5.634531
H	-0.302148	-0.632207	-5.085480

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- E 1.53 kcal/mol

C	-3.255620	-1.885425	0.604495
N	-2.062168	-1.041551	0.369977
H	-3.615581	-1.724274	1.623953
H	-4.041494	-1.614212	-0.105507
H	-2.995014	-2.938933	0.472448
H	-1.297412	-1.253444	1.057537
H	-1.686567	-1.157780	-0.597356
S	0.129988	-0.125936	3.140252
O	1.399947	0.598699	2.936396
O	-0.023470	-1.265132	2.219910
O	0.255830	-0.871334	4.583638
H	0.247630	-0.176074	5.266497
O	-1.038692	0.755875	3.240943
H	-2.270742	-0.004305	0.510959
C	3.896665	-0.071211	0.509951
N	2.437394	0.169500	0.436222
H	4.376689	0.779162	1.000887
H	4.089911	-0.978930	1.087611
H	4.300735	-0.185425	-0.499354
H	1.951575	-0.600845	-0.060080
H	2.023427	0.285363	1.399543
S	0.277952	-1.019864	-2.587905
O	-1.155417	-1.082456	-2.279219
O	1.164095	-1.483411	-1.515270
O	0.404878	-2.093598	-3.800511
H	1.326298	-2.074534	-4.117627
O	0.694645	0.284338	-3.163267
H	-0.728541	1.360607	-3.332222
O	-1.508998	1.960383	-3.222015
H	2.207162	1.033939	-0.138993
H	-2.253531	1.342907	-3.152465
O	1.729964	2.163156	-1.284860

H	1.482110	1.574164	-2.032557
H	0.882048	2.611581	-1.055264
O	-0.908020	3.109802	-0.909583
H	-1.080082	4.062193	-0.947787
H	-1.210508	2.735083	-1.796581
O	-2.384516	1.596336	0.952592
H	-1.892405	1.522242	1.803127
H	-1.857572	2.197240	0.375560

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- F 1.79 kcal/mol

C	4.069882	-0.275589	0.235659
N	2.593339	-0.175722	0.177190
H	4.501405	0.204038	-0.646776
H	4.430461	0.227150	1.136712
H	4.369577	-1.326744	0.259549
H	2.216104	-0.636119	-0.681777
H	2.146319	-0.594173	1.025908
S	0.273210	-0.983244	-2.581871
O	1.669593	-1.284270	-2.240658
O	0.108011	-0.219949	-3.818286
O	-0.472061	-2.416849	-2.813251
H	-0.082928	-2.822056	-3.609687
O	-0.496157	-0.454708	-1.431248
H	2.264066	0.841429	0.190837
C	-3.788971	-1.411615	0.331018
N	-2.491676	-0.723157	0.510956
H	-4.279840	-1.036168	-0.570853
H	-3.628256	-2.488877	0.235088
H	-4.424961	-1.214513	1.197847
H	-1.983197	-1.028214	1.378611
H	-1.848380	-0.866729	-0.292011
S	0.115127	-0.250379	2.994649
O	1.393939	-0.855577	2.589269
O	-1.034301	-1.154947	2.812086
O	0.227273	0.009718	4.596020
H	0.365973	-0.855392	5.022920
O	-0.102593	1.109139	2.477136
H	-1.723589	1.869112	1.634130
O	-2.398352	1.955259	0.927393
H	-2.590442	0.338385	0.619632
H	-1.881518	2.286889	0.151307
O	1.594650	2.328436	0.517524
H	1.096390	2.085219	1.328269
H	0.879781	2.495030	-0.147596
O	-0.604780	2.306215	-1.156893
H	-0.675647	2.612595	-2.098347
H	-0.548933	1.326708	-1.264399
O	-0.722266	2.459707	-3.876432
H	-0.442246	1.517540	-3.960101
H	-0.074294	2.960836	-4.392089

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- G 2.26 kcal/mol

C	3.618979	-1.878984	-0.221922
N	2.571989	-0.831678	-0.168315
H	4.262572	-1.702599	-1.087727
H	4.215353	-1.847069	0.693851
H	3.149550	-2.861603	-0.314368
H	1.998845	-0.849620	-1.048092
H	1.950382	-0.968310	0.661894
S	0.030373	-0.270806	-2.869386
O	1.282313	-0.998839	-2.611481
O	0.014261	0.549984	-4.061629
O	-1.132526	-1.428527	-3.061664
H	-1.008022	-1.807430	-3.950234
O	-0.488119	0.385552	-1.636212
H	2.998939	0.131715	-0.061384
C	-3.843206	-1.146984	-0.584643
N	-2.630540	-0.468044	-0.079245
H	-4.309424	-0.533782	-1.360366
H	-3.569724	-2.116271	-1.009194
H	-4.548593	-1.292136	0.237855
H	-2.151682	-0.999534	0.689013
H	-1.913493	-0.312719	-0.821682
S	-0.170447	-0.706803	2.602205
O	1.206262	-1.081661	2.245824
O	-1.211091	-1.554798	2.015845
O	-0.329192	-1.035947	4.186298
H	0.350441	-0.523776	4.661192
O	-0.418133	0.745238	2.455254
H	-1.971713	1.690787	1.774615
O	-2.625246	1.996286	1.108070
H	-2.815780	0.494389	0.332247
H	-2.080256	2.511417	0.471255
O	3.472113	1.729817	0.177498
H	2.654614	2.140770	0.609151
H	4.224869	1.999185	0.721741
O	-0.713203	2.920002	-0.784012
H	-0.738435	3.603441	-1.469090
H	-0.586150	2.055060	-1.258660
O	1.252233	2.673784	1.232300
H	0.629875	2.896043	0.503453
H	0.776855	1.980504	1.743030

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₄- H 2.91 kcal/mol

C	3.756295	1.185121	0.125199
N	2.312523	0.868626	0.207242
H	4.037408	1.316366	-0.923064
H	3.957295	2.107532	0.675958
H	4.339200	0.368182	0.559027
H	2.080407	0.034940	-0.365095
H	1.994998	0.725936	1.196246
S	0.433439	-0.661967	-2.884732
O	-0.678690	-1.584984	-2.591052
O	1.553124	-0.793385	-1.942260

O	1.004910	-1.094720	-4.344499
H	1.304490	-2.019709	-4.276089
O	0.005691	0.725618	-3.133665
H	1.700892	1.637002	-0.218694
C	-2.641778	-2.120491	0.495400
N	-1.445717	-1.353435	0.076897
H	-3.464803	-1.921718	-0.196280
H	-2.411723	-3.189079	0.489420
H	-2.925580	-1.815102	1.505984
H	-0.653156	-1.498145	0.750129
H	-1.131736	-1.596051	-0.892814
S	0.425534	-0.470124	2.984636
O	1.290995	0.709299	2.801319
O	0.592872	-1.483056	1.931469
O	0.984946	-1.257448	4.294861
H	0.870060	-0.665665	5.060553
O	-0.975473	-0.130348	3.280810
H	-1.966853	1.242358	2.815580
O	-2.582179	1.912484	2.422087
H	-1.637019	-0.313295	0.061382
H	-2.336099	2.755211	2.829529
O	-2.610700	1.539601	-2.630579
H	-3.280564	1.011655	-3.087048
H	-1.742482	1.191914	-2.949588
O	-1.779489	1.396344	-0.069473
H	-2.335204	1.556405	-0.874533
H	-2.214672	1.740302	0.759406
O	0.578613	2.564009	-0.993348
H	0.511789	2.130655	-1.871486
H	-0.271924	2.292333	-0.564917

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₅- A 0.00 kcal/mol

C	3.880975	0.134640	-0.208782
N	2.429550	0.232941	0.069556
H	4.181140	0.953616	-0.867834
H	4.435519	0.201542	0.730736
H	4.100146	-0.819783	-0.695016
H	1.868133	0.174473	-0.814407
H	2.116438	-0.511272	0.734740
S	-0.437906	0.434701	-2.304567
O	1.038138	0.188223	-2.344476
O	-0.905636	1.247778	-3.410449
O	-1.144519	-0.991674	-2.357082
H	-0.976051	-1.410902	-3.284050
O	-0.837498	0.910752	-0.949982
H	2.182530	1.138698	0.570925
C	-3.732196	-1.062943	0.469839
N	-2.447644	-0.446775	0.868852
H	-4.337385	-0.328865	-0.068795
H	-3.539214	-1.918426	-0.182469
H	-4.269841	-1.393769	1.362318
H	-1.841401	-1.094921	1.427970

H	-1.892335	-0.117591	0.047739
S	0.449794	-1.049047	2.983386
O	1.632317	-1.389545	2.177259
O	-0.756051	-1.796653	2.589611
O	0.789088	-1.515670	4.502868
H	0.930236	-2.479951	4.486600
O	0.230627	0.397959	3.150609
H	-1.437472	1.358449	2.945781
O	-2.211118	1.753429	2.486684
H	-2.556315	0.411476	1.484968
H	-1.808301	2.410689	1.876335
O	1.675543	2.329590	1.649003
H	1.276053	1.742215	2.329771
H	0.900327	2.791796	1.256412
O	-0.750476	3.161799	0.473788
H	-0.961275	3.987652	0.015213
H	-0.788345	2.439318	-0.210563
O	-0.624180	-1.985151	-4.702247
H	0.266194	-1.563617	-4.890228
H	-1.232517	-1.592092	-5.346164
O	1.746018	-0.712962	-4.830851
H	1.775254	0.036279	-5.444246
H	1.594245	-0.301814	-3.939914

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₅- B 2.68 kcal/mol

C	4.146821	0.670459	-0.134101
N	2.673884	0.529481	-0.084561
H	4.406505	1.565652	-0.705466
H	4.539695	0.761830	0.882026
H	4.585767	-0.206310	-0.617686
H	2.263378	0.439292	-1.049653
H	2.383077	-0.301768	0.477857
S	0.154091	0.234010	-2.759407
O	1.615893	0.335194	-2.622253
O	-0.360728	0.747734	-4.030080
O	-0.229940	-1.330294	-2.688156
H	-0.295834	-1.662747	-3.637493
O	-0.546537	0.766414	-1.557390
H	2.215285	1.354415	0.405253
C	-3.317670	-1.539027	-0.424371
N	-2.239490	-0.685018	0.122573
H	-3.926797	-0.953353	-1.118088
H	-2.881145	-2.389385	-0.954440
H	-3.947006	-1.898736	0.394045
H	-1.641941	-1.197179	0.811356
H	-1.612781	-0.321331	-0.628899
S	0.603246	-1.241582	2.526675
O	1.739530	-1.472652	1.625321
O	-0.641479	-1.889508	2.085995
O	0.989508	-1.944541	3.942807
H	1.086971	-2.899821	3.775430
O	0.437406	0.167202	2.930830

H	-2.689637	1.562480	2.266449
O	-3.002041	1.624197	1.324283
H	-2.618158	0.185443	0.619668
H	-2.389743	2.260368	0.894125
O	1.380273	2.414456	1.414323
H	1.045893	1.763057	2.067743
H	0.576383	2.740194	0.947037
O	-0.922430	2.983678	-0.116780
H	-1.045119	3.811088	-0.604373
H	-0.762737	2.278049	-0.799618
O	-0.523121	-1.664883	-5.316823
H	0.268883	-1.882123	-5.831003
H	-0.516822	-0.681100	-5.233347
O	-1.906506	1.319201	3.800979
H	-2.342287	0.816635	4.503532
H	-1.073513	0.827085	3.599554

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₅- C 2.76 kcal/mol

C	3.984845	0.325210	0.531212
N	2.515222	0.405695	0.366710
H	4.464328	1.016681	-0.166661
H	4.255131	0.596496	1.555161
H	4.325621	-0.691826	0.318957
H	2.231156	0.146996	-0.613501
H	2.011213	-0.208820	1.042296
S	0.521073	-0.098008	-2.744583
O	1.902759	-0.195191	-2.248312
O	0.416236	0.294178	-4.151384
O	-0.139107	-1.562700	-2.607685
H	-0.122703	-1.988253	-3.522737
O	-0.334144	0.705656	-1.826304
H	2.142161	1.379592	0.584475
C	-3.603001	-1.068848	-0.920613
N	-2.469621	-0.308709	-0.350012
H	-4.030751	-0.515799	-1.761215
H	-3.250123	-2.042128	-1.271506
H	-4.367747	-1.211758	-0.152538
H	-2.047783	-0.782146	0.488922
H	-1.704366	-0.147058	-1.040204
S	-0.402276	-0.361181	2.666726
O	0.989210	-0.817847	2.389372
O	-1.406462	-1.220326	2.017034
O	-0.599117	-0.504840	4.241115
H	-0.078562	-1.311974	4.540832
O	-0.604540	1.073356	2.401534
H	-2.094701	1.910255	1.507987
O	-2.668414	2.190996	0.761078
H	-2.732455	0.659784	-0.004560
H	-2.062463	2.721439	0.197584
O	1.341900	2.729362	1.180015
H	0.721048	2.271474	1.790902
H	0.752202	3.066217	0.467342

O	-0.538960	3.192627	-0.871553
H	-0.545092	3.899507	-1.532630
H	-0.396694	2.342382	-1.369179
O	-0.102358	-2.172243	-5.194286
H	0.676469	-2.624918	-5.550917
H	0.123404	-1.211001	-5.210987
O	1.126934	-2.532934	4.550329
H	1.372883	-2.168014	3.668897
H	0.775314	-3.417937	4.370889

(H₂SO₄)₂(CH₃NH₂)₂(H₂O)₅- D 2.82 kcal/mol

C	3.746329	-1.746834	-0.089935
N	2.518492	-0.920483	-0.053278
H	4.411967	-1.375408	-0.873537
H	4.252101	-1.688330	0.877363
H	3.483997	-2.786809	-0.301475
H	2.012413	-0.942679	-0.973565
H	1.870174	-1.228055	0.709383
S	0.086070	-0.195430	-2.871640
O	1.322598	-0.917436	-2.538720
O	-0.018459	0.193611	-4.278967
O	-1.146178	-1.187087	-2.556868
H	-1.450597	-1.578243	-3.435955
O	-0.176467	0.920290	-1.916619
H	2.726457	0.093753	0.186189
C	-3.540244	0.854958	-0.277890
N	-2.105262	0.893537	0.080077
H	-3.750073	1.622532	-1.027389
H	-3.788507	-0.127143	-0.688522
H	-4.142782	1.044822	0.614473
H	-1.865099	0.206984	0.834397
H	-1.487601	0.719891	-0.745303
S	0.066331	-0.358970	2.744256
O	0.946360	-1.386812	2.173496
O	-1.358546	-0.547523	2.337459
O	0.087646	-0.532500	4.327288
H	-0.617283	-1.207671	4.573113
O	0.545711	1.016754	2.517752
H	-0.409670	2.528629	1.823350
O	-0.888472	3.085852	1.170075
H	-1.789577	1.832551	0.468038
H	-0.209946	3.286999	0.487062
O	2.766428	1.647633	0.850772
H	2.108985	1.504177	1.568380
H	2.305103	2.249561	0.223341
O	1.071542	3.053122	-0.904848
H	1.307651	3.738588	-1.546065
H	0.690069	2.295703	-1.427363
O	-1.729132	-1.774229	-5.085072
H	-1.283899	-2.537469	-5.482595
H	-1.099480	-1.020860	-5.190684
O	-2.038872	-2.156264	4.494713

H	-2.164037	-1.739582	3.611554
H	-2.751172	-1.804952	5.049623

Methodology

At the present time, the DFT is probably the only choice for studying large pre-nucleation clusters due to prohibitively high computational expenses associated with high level *ab initio* computations with large or complete basis sets. The PW91PW91 method used in the present study has been successfully applied for studying the structural, spectroscopic and thermodynamic properties of a variety of clusters typical for the Earth's atmosphere. For example, *Ding et al.* (2003) [1] found that the Gibbs free energies of sulfuric acid hydration predicted by PW91PW91 are, in contrast to earlier B3LYP studies, consistent with atmospheric observation of stable sulfuric acid clusters found in the Earth's atmosphere. *Natsheh et al.* (2004) [2] were first to predict the anomalously high dipole of sulfuric acid hydrates $(\text{H}_2\text{SO}_4)_n(\text{H}_2\text{O})_k$, the dominant form of the gas-phase sulfuric acid in Earth's atmosphere. Two years later, such hydrates have been discovered by the group of K. Leopold of the University of Minnesota [3]

Nadykto et al. (2006) [4] have studied the thermodynamics of the water clusters using the PW91PW91 method and have solved the classical problem of the sign preference in ion-induced water vapour nucleation established in Wilson's 1897 pioneering cloud chamber experiments. *Kurten et al.* (2007) [5] and, independently, *Nadykto and Yu* (2007) [6] have used the PW91PW91 method to point out the deficiency the popular B3LYP method in describing the thermodynamics of the sulfuric acid-water and sulfuric acid-water ammonia $(\text{H}_2\text{SO}_4)_n(\text{NH}_3)_m(\text{H}_2\text{O})_k$ clusters and to resolve the B3LYP predictivity issues related to the thermochemistry of binary and ternary atmospheric clusters containing. The same PW91PW91 method was used in [7], where long standing controversies over the role of the ion sign in binary nucleation of sulfuric acid in the Earth's atmosphere have been resolved.

More recently, large $(\text{H}_2\text{SO}_4)_n(\text{NH}_3)_m(\text{H}_2\text{O})_k$ pre-nucleation clusters consisting of the sulfuric acid with other common atmospheric species such as water and ammonia has been studied using PW91PW91 method by *Herb et al.* (2013) [8]. It has been shown that PW91PW91 the Gibbs free energies are in excellent agreement with the experimental data and high level CCSD (T)/CBS method while showing no sign of deterioration with the growing cluster size and pointed out that PW91PW91 method is a viable alternative to higher level *ab initio* methods in studying large binary and ternary atmospheric pre-nucleation clusters containing H_2SO_4 , for which the higher level *ab initio* computations are prohibitively expensive.

This conclusion is fully confirmed by the comparison of the PW91PW91 data with all the high level *ab initio* studies and experimental data available at the present time. As it may be seen from Table 2S, in which the comparison of the PW91PW91 results with all the available purely experimental data for reactions involving the sulfuric acid, the key atmospheric nucleation precursor, and other relevant atmospheric species and best available *ab initio* calculations featuring virtually zero's basis set superposition error due to the application of the CBS, the PW91PW91 is in a very good agreement with both measurements and high level *ab initio* methods. The average difference between the PW91PW91 Gibbs free energies and measured values over the entire dataset does not exceed $1.26 \text{ kcal mol}^{-1}$, which is very close to the average experimental uncertainty of $1.23 \text{ kcal mol}^{-1}$ and chemical accuracy limit of $1.0 \text{ kcal mol}^{-1}$.

Table 2S. Comparison of the theoretical and experimental standard conditions $(\text{HSO}_4^-)(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_{n-1}+(\text{H}_2\text{O}) \rightleftharpoons (\text{HSO}_4^-)(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_n$ reaction Gibbs free energies. Abbreviations *best ab initio* refer to CCSD (T)/CBS (ions) ([9] and RI-MP2/CBS studies [10]) and Experiments refer to [11,12]. PW91PW91/6-311++G (3df,3pd) data are adopted from [6–8].

Reaction	ΔG (best ab initio)	ΔG (PW91)	ΔG (exp)
$(\text{HSO}_4^-)(\text{H}_2\text{O})+(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})$	-3.91	-4.58	-6.04±1.0
$(\text{HSO}_4^-)(\text{H}_2\text{O})+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_2$	-3.32	-3.42	-4.64±1.1
$(\text{HSO}_4^-)(\text{H}_2\text{O})_2+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_3$	-2.53	-2.99	-3.25±0.6
$(\text{HSO}_4^-)(\text{H}_2\text{O})_3+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_4$	-1.44	-2.98	-2.2±0.9
$(\text{HSO}_4^-)(\text{H}_2\text{O})_4+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_5$	-2.31	-1.38	-2.32±2.4
$(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})$		-0.60	-2.41±1.13
$(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_2$		-1.10	-1.60±0.60
$(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_2+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{HSO}_4^-)(\text{H}_2\text{O})_3$		-2.58	-1.10±2.08
$(\text{H}_2\text{SO}_4)_2(\text{HSO}_4^-)(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)_2(\text{HSO}_4^-)(\text{H}_2\text{O})$		-0.68	-1.00±2.01
$(\text{H}_2\text{SO}_4)_2(\text{HSO}_4^-)(\text{H}_2\text{O})+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)_2(\text{HSO}_4^-)(\text{H}_2\text{O})_2$		-1.43	-1.71±1.43
$(\text{H}_2\text{SO}_4)_2(\text{HSO}_4^-)(\text{H}_2\text{O})_2+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)_2(\text{HSO}_4^-)(\text{H}_2\text{O})_3$		-4.31	-2.09±1.06
$(\text{H}_2\text{SO}_4)_3(\text{HSO}_4^-)(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)_3(\text{HSO}_4^-)(\text{H}_2\text{O})$		-3.61	-2.72±0.60
$(\text{H}_2\text{SO}_4)_3(\text{HSO}_4^-)(\text{H}_2\text{O})+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)_3(\text{HSO}_4^-)(\text{H}_2\text{O})_2$		-1.25	-1.52±0.67
$(\text{H}_2\text{SO}_4)_3(\text{HSO}_4^-)(\text{H}_2\text{O})_2+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)_3(\text{HSO}_4^-)(\text{H}_2\text{O})_3$		-4.75	-1.92±0.46
$(\text{H}_2\text{SO}_4)+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_1$	-2.87	-2.27	-3.6±1.0
$(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_1+(\text{H}_2\text{O})\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{H}_2\text{O})_2$	-1.24	-2.99	-2.3 ±0.3
$(\text{H}_2\text{SO}_4)+\text{NH}_3\rightleftharpoons(\text{H}_2\text{SO}_4)(\text{NH}_3)_1$		-7.77	-8.0

The average difference of the high level CCSD (T)/CBS is less than 0.9 kcal mol⁻¹ while the degree of agreement of both methods with the experimental data is nearly identical. Systematic benchmarking and validation of PW91/6-311+G(3df,3pd) against experimental data and high level *ab initio* results for aqueous, binary and ternary systems relevant to atmospheric nucleation show clearly that PW91PW91 functional provides reliable Gibbs free energies, geometries, dipole moments and vibrational spectra within uncertainties of the experimental data. Being a pure GGA functional, PW91PW91 can also take advantage of the density fitting (DF), which is an important factor in the case, when very large clusters are studied. These considerations lead us to a logical conclusion that the DFT PW91PW91 method is the optimum choice for studying clusters nucleating in the Earth's atmosphere, which are investigated in the present work.

In the present study the initial/generated geometries, for each cluster class, typically over 20–50 initial geometries were sampled. The input geometries were optimized using the semi-empirical PM3. In the case of the smallest clusters a minimum of 10–20 PM3-optimized geometries were obtained. The most stable isomers located within 5 kcal mol⁻¹ of the intermediate global minimum were recomputed at the PW91PW91/6-31+G* and they were then finally optimized using the PW91PW91/6-311+G (3df,3pd).

References

1. Ding, C.G.; Laasonen, K.; Laaksonen, A. Two sulfuric acids in small water clusters. *J. Phys. Chem. A* **2003**, *107*, 8648–8658.
2. Al Natsheh, A.; Nadykto, A.B.; Mikkelsen, K.V.; Yu, F.; Ruuskanen, J. Sulfuric acid and sulfuric acid hydrates in gas phase: A DFT investigation. *J. Phys. Chem. A* **2004**, *108*, 8914–8929.

3. Brauer, C.S.; Sedo, G.; Leopold, K.R. Dipole moment of the H₂SO₄-H₂O complex. *Geophys. Res. Lett.* **2006**, *33*, L23805.
4. Nadykto, A.B.; Al Natsheh, A.; Yu, F.; Mikkelsen, K.V.; Ruuskanen, J. Quantum nature of the sign preference in the ion-induced nucleation. *Phys. Rev. Lett.* **2006**, *96*, 125701.
5. Torpo, L.; Kurten, T.; Vehkamäki, H.; Laasonen, K.; Sundberg, M.R.; Kulmala, M. Significance of ammonia in atmospheric nanoclusters. *J. Phys. Chem. A* **2007**, *111*, 10671–10674.
6. Nadykto, A.B.; Yu, F. Strong hydrogen bonding between atmospheric nucleation precursors and organic acids. *Chem. Phys. Lett.* **2007**, *435*, 14–18.
7. Nadykto, A.B.; Yu, F.; Herb, J. Towards understanding the sign preference in binary atmospheric nucleation. *Phys. Chem. Chem. Phys.* **2008**, *10*, 7073–7078.
8. Herb, J.; Xu, Y.; Yu, F.; Nadykto, A.B. Large hydrogen-bonded pre-nucleation clusters in the Earth's atmosphere. *J. Phys. Chem. A* **2013**, *117*, 133–152.
9. Husar, D.E.; Temelso, B.; Ashworth, A.L.; Shields, G.C. Hydration of the bisulfate ion: Atmospheric implications. *J. Phys. Chem. A* **2012**, *116*, 5151–5163.
10. Temelso, B.; Ngoc Phan, T.; Shields, G.C. A computational study of the hydration of sulfuric acid dimers: Implications for acid dissociation and aerosol formation. *J. Phys. Chem. A* **2012**, *116*, 9745–9758.
11. Froyd, K.D.; Lovejoy, E.R. Experimental thermodynamics of cluster ions composed of H₂SO₄ and H₂O. 2. Measurements and *ab initio* structures of negative ions. *J. Phys. Chem. A* **2003**, *107*, 9812–9824.
12. Hanson, D.R.; Lovejoy, E.R. Measurement of the thermodynamics of the hydrated dimer and trimmers. *J. Phys. Chem. A* **2006**, *110*, 9525–9538.

© 2015 by the authors; licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).