

# **Ion Mobility Spectrometry-Mass Spectrometry Examination of the Structures, Stabilities, and Extents of Hydration of Dimethylamine-Sulfuric Acid Clusters**

Jikku M. Thomas<sup>1</sup>, Siqin He<sup>2</sup>, Carlos Larriba-Andaluz<sup>3</sup>, Joseph W. DePalma<sup>4,5</sup>, Murray V. Johnston<sup>4</sup>, & Christopher J. Hogan Jr.<sup>2,\*</sup>

<sup>1</sup>Department of Chemical Engineering & Materials Science, University of Minnesota,  
Minneapolis, MN, USA

<sup>2</sup>Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN, USA

<sup>3</sup>Department of Mechanical Engineering, Indiana University-Purdue University, Indianapolis, IN

<sup>4</sup>Department of Chemistry & Biochemistry, University of Delaware, Newark, DE

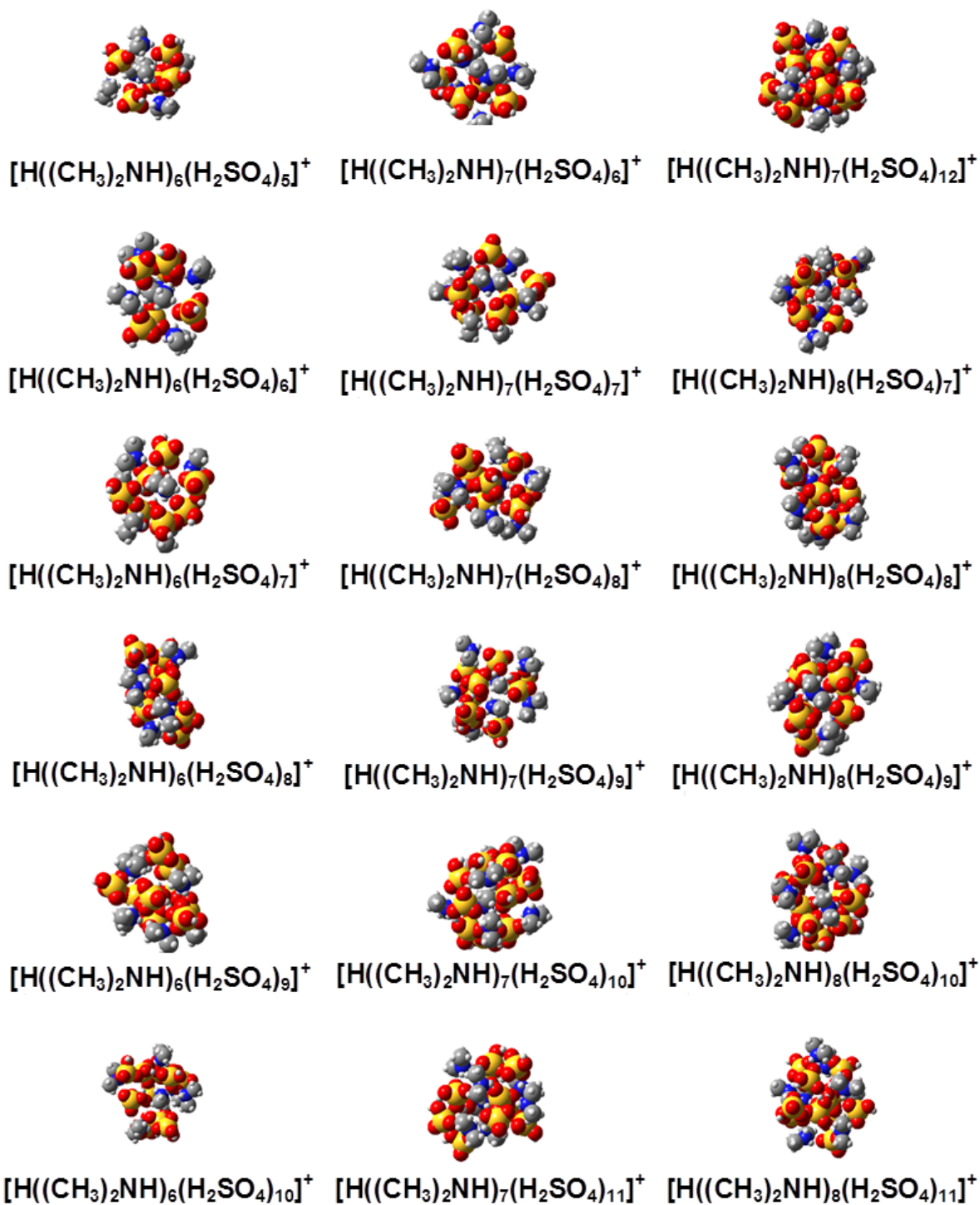
<sup>5</sup>Current Address: Department of Chemistry, Yale University, New Haven, CT

## **Supplemental Information**

**\*To whom correspondence should be addressed: [hogan108@umn.edu](mailto:hogan108@umn.edu), Tel: 1-612-626-8312, Fax: 1-612-625-6069.**

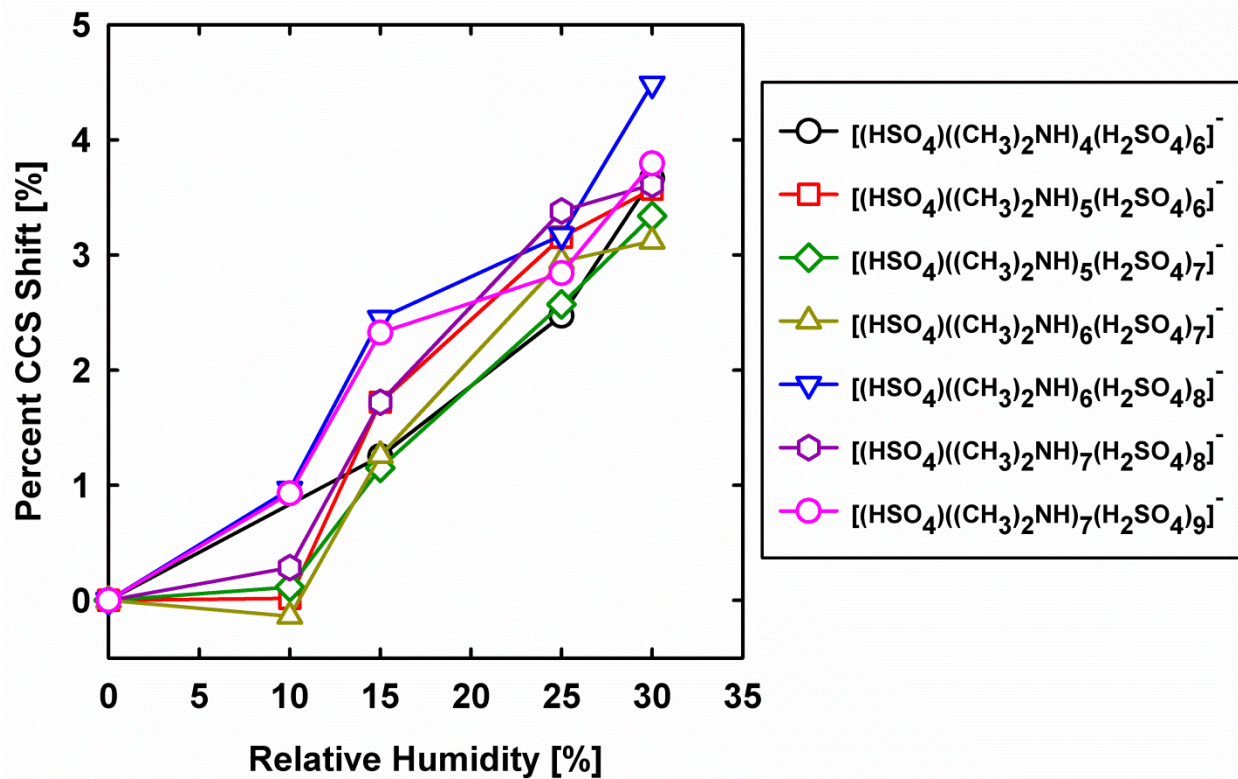
**Parameters used in the calculation of CCSs of Cluster Ions**

1. Temperature: 304 K
2. Pressure: 101,325 Pa
3. Polarizability of gas molecules:  $1.7 \times 10^{-30} \text{ m}^3$
4. Radius of gas molecules: 1.5 Å
5. Mass of gas molecules: 28.96 Da
6. Reemission law for gas molecules: Maxwell-Boltzmann distributed with a mean velocity 8 % lower than the mean velocity at the gas temperature
7. van der Waal radii of atoms in the cluster: a) hydrogen- 1 Å b) carbon- 1.7 Å  
c) nitrogen- 1.55 Å d) oxygen- 1.52 Å e) sulfur- 1.8 Å
8. Simulation parameters: a) time step- 450 b) domain size- 16 Å c) number of gas molecules- 300000 d) number of rotations- 3



**Figure S1.** Depictions of local energy minimum positively charged dimethylamine-sulfuric acid cluster structures, which were used in gas molecule scattering calculations for collision cross section prediction.

Negative Cluster Ion Collision Cross Section Shifts



**Figure S2.** The inferred shifts in collision cross sections with change in relative humidity for negatively charged cluster ions.

### Dimethylamine-Sulfuric Acid Cluster Ion Structures

These geometries were computed using the PM6 semi-empirical method (the best available for weakly bound systems). The optimizations were performed using Gaussian 09 at 304 K and 1 atm pressure. All structures are local energy minimum geometries (no negative or imaginary vibrational frequencies).

**Cartesian coordinates for cluster ions shown in article Figure 6, in Å.**



S	3.1258890	2.3476740	1.4404900
O	4.4433640	1.7788600	1.0812270
O	2.3657880	2.9014060	0.2995420
O	3.5484460	3.7106750	2.3390430
O	2.3178390	1.5040330	2.3222140
H	4.4966440	3.8259490	2.4945660
S	-1.8097310	-2.1793130	1.7746550
O	-1.1770600	-1.8081780	0.4862150
O	-0.8054820	-2.7586420	2.7263670
O	-2.8119170	-3.4436570	1.4369130
O	-2.5495830	-1.0784200	2.4271450
H	-3.4280450	-3.2791700	0.6445380
S	3.3375970	-2.3250750	-1.5535080
O	2.3681110	-3.4207240	-1.5598910
O	3.0928600	-1.2930120	-0.4976360
O	2.9344710	-1.4309270	-2.9383060
O	4.7536750	-2.6317930	-1.6750660
H	2.9822350	-1.8960500	-3.7821710
S	-2.6934470	-1.0233450	-1.3943220
O	-1.3904100	-1.5345040	-1.8924710
O	-3.4087080	-1.9547900	-0.4798370
O	-3.6708110	-0.8775870	-2.7079100
O	-2.6489020	0.3524750	-0.8057660
H	-3.7055830	0.0706880	-3.0955910
S	-2.7701820	2.5365640	-1.6359540
O	-1.3064240	2.6437060	-1.3430820
O	-3.1786680	1.7033560	-2.7736320
O	-2.9307550	4.1134540	-2.2813290
O	-3.6441110	2.5625710	-0.4483640
H	-3.5688140	4.2112790	-2.9956820
N	-4.4837240	0.6455310	1.2174190
C	-5.6034360	-0.2931160	0.8726650
C	-4.9439850	1.7650100	2.1080650
H	-5.1999390	-1.1552190	0.2846240
H	-6.0929270	-0.7073230	1.7679270

H	-6.3700190	0.1988500	0.2506120
H	-4.1472750	2.5329180	2.1719850
H	-5.8230440	2.2822250	1.6797670
H	-5.1989050	1.4151950	3.1189840
H	-3.6992870	0.1008930	1.6840950
H	-4.0538590	1.0798490	0.3023030
N	0.1102210	-1.1104290	4.5867490
C	-1.1495610	-0.4646180	5.0946190
C	1.0172320	-0.1218480	3.9144870
H	-1.7064350	-1.1541510	5.7538870
H	-0.9602890	0.4704800	5.6441850
H	-1.8353640	-0.2344990	4.2389790
H	1.9538380	-0.5953310	3.5642070
H	0.5556690	0.3259870	2.9997110
H	1.3043460	0.7307020	4.5536880
H	0.6095840	-1.5643890	5.3710800
H	-0.1762920	-1.9128380	3.8558210
N	-0.3665480	-3.9404060	-1.2600720
C	-0.4362270	-4.9169120	-0.1207770
C	-1.1281500	-4.4210750	-2.4642510
H	0.2064300	-4.5748630	0.7156780
H	-1.4664120	-5.0024930	0.2830560
H	-0.0938130	-5.9229150	-0.4142920
H	-1.2125440	-3.5872860	-3.1971730
H	-0.6318580	-5.2735460	-2.9544190
H	-2.1598590	-4.7192590	-2.2064290
H	-0.7670510	-2.9778670	-0.9537070
H	0.6494560	-3.7736410	-1.5253530
N	5.6350290	-0.2334100	0.1093310
C	6.2718980	-1.4679730	0.6832830
C	6.1824910	0.0723740	-1.2579340
H	5.8269440	-1.7181680	1.6608860
H	6.1060220	-2.3438700	0.0052220
H	7.3601950	-1.3542560	0.8123860
H	5.6630570	0.9474010	-1.6897570
H	7.2624560	0.2895410	-1.2340160
H	6.0272810	-0.7924860	-1.9464130
H	4.5725230	-0.3739290	0.0425910
H	5.7772100	0.5942320	0.7499190
N	0.4154440	4.3350380	-0.9268930
C	1.5044870	4.6348240	-1.9184330
C	0.3305580	5.3847570	0.1442410
H	1.4277550	3.9534890	-2.7853640
H	1.4549770	5.6694210	-2.2942120
H	2.5016160	4.4717780	-1.4540440
H	-0.5147360	5.1688020	0.8242030

H	1.2562700	5.4051860	0.7549820
H	0.1717190	6.3928120	-0.2751790
H	-0.5309150	4.2171090	-1.4227810
H	0.6132450	3.3886590	-0.4735070
N	0.6613740	0.0439340	-0.6010320
C	1.0330870	0.8311660	-1.8282830
C	0.0527470	0.9217260	0.4586940
H	1.4226070	0.1530170	-2.6149560
H	0.1433520	1.3668500	-2.2307780
H	1.8147960	1.5783620	-1.5984450
H	0.2998410	0.5524250	1.4723910
H	0.4114820	1.9691150	0.3842550
H	-1.0566890	0.9651950	0.3302180
H	-0.0419920	-0.7149930	-0.8698490
H	1.5252020	-0.4380660	-0.2241520

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>6</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>6</sub>]<sup>+</sup>**

S	3.2677620	2.7583010	0.5901710
O	4.2218020	2.3191980	-0.4253460
O	1.9559670	3.2099410	0.1267420
O	3.9822810	4.1095530	1.2772840
O	3.1825350	1.7947400	1.7436190
H	4.8576210	4.3473860	0.9295980
S	3.2683490	-0.3257350	2.3745590
O	4.2063680	-0.4466440	1.2931840
O	1.8405410	-0.3874140	2.2324970
O	3.8173230	0.5845170	3.6256770
O	3.4962250	-1.7359310	3.3136600
H	3.8063370	1.5843660	3.4704030
S	-1.7845800	-2.7252940	1.0770160
O	-1.4939350	-1.8919020	-0.1148440
O	-0.6099910	-3.5717760	1.4543470
O	-2.9018660	-3.8387360	0.5867850
O	-2.2866560	-1.9735890	2.2477570
H	-3.7040560	-3.4373740	0.1097860
S	2.5037800	-1.6937000	-3.1070800
O	1.5397690	-2.7850770	-3.2669180
O	2.4241680	-1.0073370	-1.7800270
O	1.8843180	-0.4694080	-4.1065930
O	3.8783850	-1.8969500	-3.5282650
H	1.8929630	-0.6406060	-5.0551660
S	-3.3961400	-0.6732780	-1.2643420
O	-2.3022590	-1.0172090	-2.2002950
O	-3.8936520	-1.7965670	-0.4264780
O	-4.6764170	-0.2214550	-2.1962850

O	-3.1415310	0.5364570	-0.4116000
H	-4.8741530	0.7824890	-2.1818520
S	-3.4851810	2.7944340	-0.4877860
O	-2.0426250	2.8083100	-0.9088710
O	-4.4757890	2.3471200	-1.4690240
O	-3.7130140	4.5029410	-0.5146680
O	-3.7032510	2.4854720	0.9351500
H	-4.5289610	4.7983730	-0.9329440
N	-4.1757460	0.1198010	2.1495960
C	-5.5182460	-0.4601110	1.8064590
C	-4.2371520	0.9922540	3.3722320
H	-5.4084030	-1.1572980	0.9386740
H	-5.9525060	-1.0345610	2.6387660
H	-6.2346440	0.3254500	1.5096370
H	-3.2166000	1.2550260	3.7003360
H	-4.7400790	1.9526320	3.1277530
H	-4.7667870	0.5123760	4.2080670
H	-3.4754380	-0.6711280	2.2877590
H	-3.8157020	0.7275740	1.3116340
N	0.7723350	-2.9676940	3.6562570
C	0.7002460	-4.1709030	4.5530730
C	0.0075080	-1.8002150	4.2144950
H	1.2340390	-5.0249490	4.0940680
H	1.1404630	-3.9831920	5.5466090
H	-0.3492560	-4.4931070	4.7016950
H	0.2843130	-0.8747360	3.6587130
H	-1.0888880	-1.9351820	4.0590070
H	0.1987010	-1.6315980	5.2831670
H	1.7736610	-2.6894980	3.5098550
H	0.3421960	-3.2293550	2.6667780
N	-1.0795620	-3.4015050	-2.5168780
C	-0.9417850	-4.6677000	-1.7208240
C	-2.0372330	-3.5559020	-3.6661100
H	-0.1950580	-4.5314950	-0.9096270
H	-1.8943420	-4.9476040	-1.2255660
H	-0.6087680	-5.5138080	-2.3434830
H	-2.2843100	-2.5476180	-4.0689890
H	-1.6108910	-4.1668140	-4.4775770
H	-2.9915070	-4.0113560	-3.3498880
H	-1.4271490	-2.5939730	-1.8790150
H	-0.1239790	-3.1102210	-2.8886430
N	5.0259550	-0.0894480	-1.2075500
C	5.7742500	-1.3873420	-1.0788890
C	5.3878810	0.6314560	-2.4771440
H	5.4834600	-1.8918170	-0.1365490
H	5.5239040	-2.0652380	-1.9281610



H	6.8650030	-1.2413570	-1.0737400
H	4.8436800	1.5987350	-2.5194500
H	6.4651480	0.8491450	-2.5379420
H	5.1091370	0.0248370	-3.3671370
H	3.9747640	-0.2908610	-1.1951570
H	5.2048850	0.5293910	-0.3773600
N	-0.4023490	4.7683430	-0.1980650
C	-0.1433040	5.6859530	-1.3590720
C	-1.1467380	5.4659990	0.9046640
H	0.4072030	5.1459150	-2.1520630
H	-1.0943340	6.0427470	-1.8005960
H	0.4521660	6.5686800	-1.0725490
H	-1.2200230	4.8120380	1.7924290
H	-0.6759580	6.4131990	1.2075790
H	-2.1969800	5.6791500	0.5875670
H	-1.0230450	3.9055180	-0.5466360
H	0.5107140	4.3797180	0.1589580
N	0.1021150	0.2769420	-1.0239480
C	0.2232100	1.3573960	-2.0632750
C	-0.1691300	0.8452130	0.3410690
H	0.5229680	0.9221340	-3.0379770
H	-0.7525030	1.8818970	-2.1931410
H	0.9741050	2.1132370	-1.7742390
H	-0.0170750	0.0721520	1.1160950
H	0.4927420	1.6975980	0.5741730
H	-1.2233350	1.2069920	0.4000460
H	-0.6918150	-0.3795570	-1.2900850
H	0.9938240	-0.2950140	-1.0041790
H	4.2428400	-1.7228140	3.9341080

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>6</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>7</sub>]<sup>+</sup>**

S	2.0526310	4.3726290	0.2657190
O	3.4178980	4.7701440	0.5211970
O	1.9426140	3.5681050	-0.9934990
O	1.2125030	5.8062960	-0.0915590
O	1.2142450	3.8489870	1.3571150
H	1.7448120	6.5287120	-0.4528320
S	0.7199790	-3.9096610	1.3892580
O	1.9543210	-4.0078090	0.5674810
O	0.6369550	-2.7983580	2.3309280
O	0.7780500	-5.3036360	2.3193530
O	-0.5135810	-4.0820360	0.5793180
H	1.6292930	-5.7662010	2.3459260
S	-3.8874960	0.5481730	1.7169950
O	-4.1430290	-0.7741390	2.2576570

O	-4.6496410	1.1576870	0.6543920
O	-2.3315500	0.9552920	1.7055070
O	-4.2036100	1.5398570	3.0499340
H	-1.7682890	0.7523100	0.8035610
H	-4.4933380	1.0765920	3.8530840
S	2.6867200	-2.5573880	-1.1315960
O	1.6627610	-3.2309310	-1.9059970
O	2.2489110	-1.6858920	-0.0676390
O	3.5636390	-1.7058290	-2.2393600
O	3.9086800	-3.5969560	-0.7281570
H	4.5359850	-1.5663430	-1.9795780
H	3.6527210	-4.3321250	-0.1009630
S	-3.3117120	-1.3535160	-1.2496730
O	-3.2635470	-2.8188860	-1.0374230
O	-4.4660900	-0.7737460	-1.9250750
O	-2.0058530	-1.1351910	-2.2379460
O	-3.0192980	-0.6705630	0.0695450
H	-1.8839640	-0.1828740	-2.6004410
S	-1.4408200	2.2649320	-1.4034500
O	-2.1401260	3.4887200	-0.9441910
O	-0.8716770	1.5288880	-0.2456480
O	-0.1925880	2.6923780	-2.3550660
O	-2.3168100	1.4001000	-2.2504270
H	0.6526760	3.0512430	-1.8725050
S	5.4198270	-0.0829170	0.5736730
O	5.7228130	-0.6082490	1.8835000
O	4.1363270	0.6969430	0.5006290
O	4.9387920	-1.5201070	-0.2841140
O	6.4196920	0.4994540	-0.3003190
H	5.3633570	-2.3475550	0.0205570
N	4.2438790	2.3516390	-1.6715600
C	4.6083620	1.3810430	-2.7598800
C	5.3912450	3.2652980	-1.3404720
H	3.8192080	0.6103150	-2.8774770
H	4.7548990	1.8798840	-3.7306310
H	5.5541810	0.8493870	-2.5066750
H	5.0935140	3.9735300	-0.5291780
H	6.2621290	2.6805990	-0.9627190
H	5.7243080	3.8552150	-2.2059160
H	3.3926130	2.9160270	-1.9420010
H	3.9721210	1.7980350	-0.7801790
N	-1.4625800	4.4765800	1.5635680
C	-1.3964200	5.9778230	1.5341140
C	-2.2756390	3.9675140	2.7172120
H	-0.6940710	6.3024070	0.7282550
H	-2.3800010	6.4302830	1.3306780

H	-1.0096810	6.3933320	2.4801520
H	-2.2804570	2.8498990	2.7197760
H	-1.8711510	4.2978180	3.6877850
H	-3.3312440	4.2845310	2.6588330
H	-1.8790400	4.1217480	0.6370730
H	-0.4621260	4.0822170	1.6240780
N	-2.8987740	-3.1919110	1.7365310
C	-2.3950270	-3.2242730	3.1520750
C	-4.1532460	-4.0027340	1.5616310
H	-1.3978560	-2.7275630	3.2150270
H	-3.0814560	-2.6826340	3.8282270
H	-2.2694570	-4.2532620	3.5280750
H	-4.4345000	-4.0073840	0.4832330
H	-4.0208730	-5.0472260	1.8845510
H	-4.9954080	-3.5632890	2.1265770
H	-3.1043670	-2.1796170	1.4653790
H	-2.1471890	-3.5512270	1.0682330
N	-5.0893730	1.6842810	-2.1013920
C	-5.1327060	3.1687390	-1.8796910
C	-6.2149150	1.2039010	-2.9748740
H	-4.2054000	3.5003670	-1.3453890
H	-5.1737000	3.7298520	-2.8273150
H	-5.9933550	3.4643480	-1.2578890
H	-6.1429780	0.0938970	-3.0757700
H	-7.2011030	1.4363800	-2.5411900
H	-6.1674420	1.6381060	-3.9864090
H	-4.1572550	1.4072100	-2.5334160
H	-5.1245710	1.1715560	-1.1704930
N	-0.9403800	-4.1463380	-2.0313140
C	-0.7752710	-3.6454620	-3.4390880
C	-0.9436580	-5.6481520	-1.9592530
H	-1.0040600	-2.5555900	-3.4736020
H	0.2775260	-3.7578480	-3.7716320
H	-1.4383750	-4.1576520	-4.1505530
H	-0.9900080	-5.9617880	-0.8947390
H	-1.8067880	-6.0836940	-2.4879790
H	-0.0202670	-6.0752520	-2.3907300
H	-0.1400100	-3.7763160	-1.4361540
H	-1.8399400	-3.7646630	-1.6052070
N	2.0185730	-0.1999520	2.0381540
C	2.8766070	-0.1882590	3.2731450
C	0.9101620	0.8071700	2.1144460
H	2.3584280	-0.6384230	4.1340470
H	3.8201520	-0.7569780	3.0970860
H	3.1885080	0.8359040	3.5446800
H	0.3277220	0.8088120	1.1612480

H	0.2068840	0.5974380	2.9330440
H	1.2902540	1.8448420	2.2271030
H	2.6278850	0.0047330	1.1753330
H	1.6116700	-1.1680010	1.8979620

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>6</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>8</sub>]<sup>+</sup>**

S	-1.8241190	-0.4097560	2.3070640
O	-2.2976870	0.2962000	1.1210010
O	-2.8468750	0.2014460	3.5158030
O	-0.4867130	-0.0139130	2.8229870
O	-1.9817020	-1.8717210	2.3342670
H	-2.3937800	0.6104030	4.2699210
O	-4.0641120	-2.5012380	-0.6407190
S	-3.5009400	-2.3488490	-1.9854220
O	-2.6484850	-1.2465450	-2.3448820
O	-4.4351970	-2.9504750	-3.1820810
O	-2.4703260	-3.6796890	-1.9751490
H	-1.5064830	-3.4759470	-2.1672670
H	-5.4589450	-1.5552430	0.1941530
S	-5.7461110	0.1210010	-1.3202270
O	-7.0161870	0.6297310	-1.7334360
O	-4.7159270	1.1238290	-0.9404730
O	-5.1353270	-0.9701660	-2.1806640
O	-5.9606380	-0.6957260	0.1365720
N	2.8615540	2.0935660	1.4201340
H	3.2670090	2.0517060	0.4373540
H	3.5032990	1.5345120	2.0352530
C	2.8156500	3.5174430	1.9013980
H	3.7302030	3.7866070	2.4499440
H	2.7046480	4.2335900	1.0542740
H	1.9392260	3.7161050	2.5663220
C	1.5053480	1.4482450	1.4043620
H	0.8204600	1.9565010	0.6878410
H	1.5693770	0.3922240	1.0765040
H	1.0054600	1.4780650	2.3938960
O	-1.2958280	5.6376110	0.8811210
H	-0.7859380	6.3242710	1.3413990
S	-1.1446240	4.0779830	1.4729200
O	-2.4800080	3.6587750	1.8865250
O	-0.0931000	4.1428640	2.4687260
O	-0.7160410	3.3252030	0.2206460
H	-0.3024220	3.8883980	-1.0929520
H	-4.2158380	1.4259610	0.8372250
N	-4.5898970	2.0053440	1.6548530
H	-3.7523210	2.2929800	2.2271740

C	-5.5163280	1.1599230	2.4832510
H	-6.1245630	1.7577500	3.1789230
H	-6.2056790	0.5694940	1.8373560
H	-4.9328380	0.4293190	3.0832030
C	-5.2725110	3.2342290	1.1134090
H	-5.9445610	3.7021340	1.8491280
H	-4.5044090	3.9894570	0.8396240
H	-5.8543490	2.9922270	0.2025220
S	1.8570920	3.6293560	-1.8415720
O	0.2677810	3.7337560	-2.0149340
O	2.3576470	4.6325820	-0.9524990
O	2.2708840	3.8837590	-3.3888560
O	2.1897510	2.2398410	-1.4502100
H	3.0141830	3.2974940	-3.7591420
H	-5.2398350	-2.3751030	-3.4062960
N	-2.0076490	1.3364020	-1.3497830
H	-2.7623210	0.6239920	-1.1397930
H	-1.8391160	1.8791540	-0.4612270
C	-2.4895400	2.2594550	-2.4358750
H	-1.7637160	3.0716770	-2.6334830
H	-2.6557790	1.7109180	-3.3804050
H	-3.4636270	2.7014370	-2.1422580
C	-0.7407060	0.6308310	-1.7431450
H	-0.9008970	-0.0077830	-2.6349790
H	0.0782540	1.3413120	-1.9533880
H	-0.4149700	-0.0393820	-0.9212860
S	3.8829170	0.8059790	-2.1655510
O	5.2536250	-0.0244190	-2.7788850
O	3.9029210	1.9951250	-3.0059760
O	2.8956940	-0.2750860	-2.3190670
O	4.3183560	0.9706040	-0.7185330
H	5.0230870	-0.1306150	-0.1063150
H	5.9209610	0.5373570	-3.2022210
S	5.7475370	-0.6579000	2.0336620
O	4.6480900	0.1534480	2.5259720
O	5.4949590	-0.9545480	0.4837400
O	5.4323910	-2.1821460	2.6458100
O	7.1077890	-0.3745510	2.3219710
H	6.2162040	-2.7303810	2.8455360
N	1.3336740	-1.9493270	3.3899900
H	1.4998850	-2.3426060	2.3990880
H	0.7928200	-1.0244730	3.2717330
C	2.6478500	-1.6986160	4.0666160
H	2.5361110	-1.4831110	5.1415310
H	3.3398500	-2.5558310	3.9558110
H	3.1613030	-0.8218260	3.6064200

C	0.4728600	-2.9177370	4.1536090
H	-0.5327160	-2.9692150	3.6714180
H	0.9058760	-3.9321260	4.1521960
H	0.3236520	-2.6050760	5.2000740
H	-2.5587110	-3.2206560	1.2508670
N	-2.4466940	-4.2089910	0.8646460
C	-1.4109620	-4.9553380	1.6566060
H	-1.2312390	-5.9633270	1.2470710
H	-0.4378510	-4.4052720	1.6230030
H	-1.7027380	-5.0571280	2.7139150
C	-3.7736960	-4.9156510	0.8931790
H	-4.5275010	-4.3038830	0.3396070
H	-3.7261410	-5.9010950	0.4009160
H	-4.1478560	-5.0517230	1.9203040
H	-2.1169730	-4.0930460	-0.1472920
N	4.0761060	-2.8748160	-2.7036580
H	3.4142270	-2.0703010	-2.4589050
C	5.2515220	-2.8510270	-1.7670890
H	4.9029970	-2.8753110	-0.7122560
H	5.9345760	-3.6980780	-1.9282130
H	5.8350570	-1.9073450	-1.8741430
C	4.5042480	-2.7512760	-4.1387130
H	5.1876080	-3.5611940	-4.4436100
H	3.6261970	-2.7679040	-4.8107560
H	5.0274100	-1.7835360	-4.3051900
H	3.5189520	-3.7530220	-2.5542640
H	1.7097090	-0.8216960	-1.0708360
S	1.0449880	-2.9217400	-0.3831090
O	2.1058840	-3.3135730	-1.3215280
O	-0.3319530	-3.1967580	-0.8172660
O	1.2140740	-1.2529420	-0.3013740
O	1.2507110	-3.3121700	1.0341180



H	0.8807130	2.0782300	4.8390270
S	1.4921060	2.1856920	2.6681770
O	2.4441560	3.2219120	2.1043690
O	0.1529350	2.2914260	2.0796890
O	1.4620790	2.6399050	4.2528120
O	2.0893350	0.8321310	2.5712750
H	3.5599810	0.0540190	2.0779720
N	4.5362660	-0.2311210	1.7255550
H	4.3673000	-0.8207180	0.8616370
S	2.9625320	4.2583970	0.2681790
O	3.4763360	2.9624880	-0.1510250

O	3.7463160	5.2380920	-0.8676700
O	1.5795110	4.6116470	0.1538020
H	4.1238890	6.0708340	-0.5355230
O	3.7841550	4.9953090	1.4861390
H	3.5551010	4.6685970	2.4173220
H	-0.7831960	2.7518400	0.1090910
N	-1.4592030	3.5580880	-0.0225030
H	-2.4150620	3.1156290	-0.1444330
H	2.9928080	0.9933520	-3.1004140
H	3.0172100	1.8605360	-1.6580140
N	3.5069830	1.7619250	-2.5983050
S	4.3985360	-2.5447060	-1.8495640
O	5.2143000	-3.8921190	-1.3691170
O	3.1969190	-2.7796510	-2.6037520
O	5.5789860	-2.2496910	-3.0128170
O	4.5439670	-1.3700600	-1.0011700
H	6.2113780	-2.9739420	-3.1781620
H	4.7839120	-4.4137350	-0.6180470
H	-1.9833190	2.0270340	-2.7095380
S	-0.2036080	0.6678550	-2.2126980
O	1.1906080	1.0853350	-2.4622090
O	-0.5392270	-0.6548530	-2.7625490
O	-1.1046060	1.7765620	-3.1031480
O	-0.6862830	0.9176940	-0.8420030
H	-3.7118140	-0.6924240	-1.7861930
N	-3.7414670	-1.6490150	-2.2435030
H	-3.0368200	-2.2700360	-1.7149000
S	-1.6446170	-3.4140940	0.4445960
O	-2.8728220	-3.6296060	1.2238370
O	-0.5248710	-4.3304280	0.7183620
O	-1.1942460	-1.8843490	0.9501910
O	-1.8958370	-3.2879370	-1.0271920
H	-0.2530320	-1.6047750	0.6523920
H	-0.5696200	-2.9052790	-2.2733340
N	0.3935400	-3.2334150	-2.5869950
H	1.0873110	-2.6725080	-2.0194100
S	2.1901910	-2.9522660	0.7582420
O	3.3091280	-3.3680650	-0.1827150
O	2.7110630	-1.9401210	1.6954440
O	1.8581280	-4.2996100	1.6046630
O	1.0046880	-2.5477690	-0.0317110
H	0.8729800	-4.6053250	1.5847950
S	-3.8004060	0.7405730	0.8686950
O	-2.9750410	1.8970480	1.2570440
O	-4.3793410	-0.0790910	1.9312660
O	-2.8937760	-0.2772760	-0.0799490

O	-4.8238220	1.1558230	-0.1756040
H	-1.8789700	-0.2772940	0.1033680
S	-0.6410540	-0.4130630	3.1892470
O	-1.5602240	-1.2844710	3.8773110
O	-1.4629330	0.2734750	1.9685730
O	0.5275720	-1.2829300	2.4749700
O	0.0351230	0.6619750	3.9101290
H	1.4992560	-0.8577740	2.4806590
H	-1.2450280	1.2958810	1.7845970
S	-4.9025210	2.0782260	-2.1908530
O	-3.5952450	2.6078930	-1.8381760
O	-5.3863470	3.0283480	-3.4793850
O	-6.1755450	2.6379660	-1.3114540
O	-5.0042740	0.7185850	-2.6552420
H	-6.2662500	2.2389880	-0.3842020
H	-6.2321940	3.5060090	-3.3692840
N	-4.0566840	-2.2899870	3.3137500
H	-3.6437870	-2.5921410	2.3694290
H	-3.6968950	-1.3131320	3.4779630
C	-5.5576610	-2.2747530	3.2300820
H	-5.8719010	-1.4880830	2.5035650
H	-5.9523220	-3.2440490	2.8852120
H	-6.0248530	-2.0287290	4.1969140
C	-3.5677780	-3.2176240	4.3912600
H	-3.7553910	-4.2723640	4.1263020
H	-2.4653900	-3.0944980	4.5106060
H	-4.0292150	-3.0048380	5.3674920
C	-1.0962190	4.3582890	-1.2410710
H	-1.8034710	5.1866080	-1.4088550
H	-0.0762850	4.7876380	-1.1443420
H	-1.1205870	3.7195460	-2.1490530
C	-1.4465850	4.4135850	1.2159160
H	-2.1700580	5.2376880	1.1567400
H	-1.7013820	3.7761960	2.0931540
H	-0.4321310	4.8255360	1.3929830
C	5.3334980	0.9900460	1.3757430
H	6.2665790	0.7366090	0.8493930
H	4.7287550	1.6594130	0.7131500
H	5.5873460	1.5863700	2.2686440
C	5.2145000	-1.0675540	2.7755470
H	4.5637850	-1.9420830	3.0114060
H	6.1905540	-1.4482290	2.4363640
H	5.3621770	-0.5063520	3.7132860
C	4.9462270	1.3934990	-2.3879790
H	5.0204650	0.4364280	-1.8148140
H	5.4868930	1.2517610	-3.3378740



H	5.4716850	2.1672670	-1.7982680
C	3.3592050	3.0501060	-3.3615500
H	3.8805020	3.0240200	-4.3313760
H	2.2824990	3.2409200	-3.5555030
H	3.7529000	3.9123710	-2.7811100
C	-5.1331860	-2.2020910	-2.1066200
H	-5.2501180	-3.1612920	-2.6344830
H	-5.3718530	-2.3659650	-1.0399280
H	-5.8765210	-1.4803240	-2.5078130
C	-3.3330940	-1.5153380	-3.6830270
H	-2.2710210	-1.1722050	-3.7361640
H	-3.4132190	-2.4673520	-4.2262500
H	-3.9560580	-0.7579610	-4.2000430
C	0.5708320	-4.6940990	-2.2751260
H	0.3545920	-4.8724320	-1.1924840
H	-0.1215320	-5.3260620	-2.8513090
H	1.6066190	-5.0202930	-2.4715480
C	0.6033020	-2.9478940	-4.0480840
H	0.0026150	-3.6052440	-4.6916030
H	0.3167820	-1.8922170	-4.2577320
H	1.6729590	-3.0625360	-4.3162200

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>6</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>10</sub>]<sup>+</sup>**

S	0.1532980	-3.1136080	3.8289690
O	1.4412890	-3.5937880	3.4059360
O	-0.5456010	-4.3909250	4.6827220
O	-0.8962450	-2.7945190	2.8990340
H	-0.3871910	-4.4047040	5.6452200
O	0.1785370	-2.2157200	5.2012640
H	0.6176840	-1.3093430	5.1380540
N	-3.1448670	-3.7212060	1.8171500
H	-2.2679090	-4.0030600	1.2972550
H	-3.0092310	-2.7055670	2.0892660
S	-0.0365160	-4.4293510	-1.2330680
O	0.9130820	-4.7616990	-0.1647860
O	0.1036210	-3.0089600	-1.7118580
O	-1.5300590	-4.4263150	-0.4516890
O	-0.1553600	-5.3235990	-2.3708220
H	-2.3065570	-4.2247780	-1.0659820
N	3.0088650	-4.1197130	1.3365560
H	2.0672670	-3.8679730	0.9019790
H	3.1101260	-3.4964990	2.1761810
N	-0.2792630	-2.6723130	-4.4414340
H	-0.9666270	-1.8957280	-4.6226350
H	-0.2097220	-2.7523260	-3.3579770

S	-3.5128830	-2.0475120	-2.8188380
O	-3.4420920	-3.1708440	-1.8766370
O	-4.5245360	-1.0420370	-2.4766390
O	-4.0226300	-2.6980880	-4.2828110
O	-2.1754660	-1.5223020	-3.1858000
H	-4.9467230	-2.5272780	-4.5269570
S	4.5354300	0.7892230	-0.7799270
O	5.8230290	1.2598460	-0.2807500
O	4.3292230	1.0912360	-2.2322560
O	3.3314190	1.7510080	-0.1239550
O	4.1643520	-0.6000650	-0.4308730
H	3.1669340	1.6405290	0.8686640
H	3.3724100	3.5608660	-1.6854640
N	2.8661410	4.2473360	-1.0621040
H	2.3586770	3.6728660	-0.3358870
H	0.6914310	1.6860040	2.2116360
S	-0.5211170	3.3221170	1.1214540
O	-1.7336310	3.9988420	1.5389140
O	-0.1291210	2.3568590	2.3438960
O	0.6199430	4.0625150	0.6326740
O	-0.8835450	2.2742370	-0.0554270
H	-1.7609050	1.6562510	0.0635230
H	-0.6160610	-1.2679600	-1.9418510
N	-0.3447910	-0.3227590	-1.5375620
H	-0.9977260	-0.1463610	-0.7311600
S	-3.8498010	0.2190020	0.8958050
O	-2.5903920	0.4073430	0.0847380
O	-3.9671640	-1.1218030	1.4444290
O	-5.0611450	0.3750790	-0.2517020
O	-4.0864470	1.3645660	1.7771500
H	-4.9489950	-0.1764570	-1.1184590
H	3.2543050	-1.2067740	0.7072810
S	2.2730770	-0.4502540	2.6502740
O	1.1790660	-1.1128500	3.4107520
O	1.8204090	0.7335150	1.8384380
O	2.6462290	-1.5626090	1.4820270
O	3.4902180	-0.1855640	3.3947750
H	-4.7419390	3.3059570	1.8092820
N	-4.2330820	3.7033180	2.6523720
H	-3.2541350	3.3203840	2.6013490
S	-7.0355950	3.6260410	-0.3709000
O	-6.2130020	3.9650760	0.7665420
O	-6.2229250	2.5699240	-1.2920260
O	-7.6482820	4.6036190	-1.1986230
H	-5.8034550	1.7465390	-0.8320050
O	-8.2258370	2.6307880	0.2197580

H	-9.0798330	2.6343470	-0.2537690
S	6.2152310	2.3781760	1.9419760
O	6.4275370	2.5856270	3.3368670
O	4.9038010	1.3259510	1.8508140
O	5.8993390	3.4660430	1.0580470
H	4.7006350	0.8356570	2.7299680
O	7.4861270	1.4911320	1.4195650
H	7.4617860	1.1982640	0.4604060
S	3.1205300	1.5728950	-4.1215470
O	2.3286370	0.3992330	-3.8504230
O	2.7670220	1.9315600	-5.7172440
O	2.8946490	2.7959910	-3.3910950
H	3.5328380	2.0859180	-6.3049940
O	4.6894370	1.3021090	-4.5171020
H	5.3158790	1.1181170	-3.7429820
C	1.0670540	-2.3213320	-5.0036430
H	1.4676100	-1.3975390	-4.5182560
H	1.8043130	-3.1225480	-4.8164420
H	1.0330820	-2.1366930	-6.0894960
C	-0.8187130	-3.9627010	-4.9947080
H	-0.4291770	-4.8363620	-4.4120440
H	-1.9236820	-3.9926600	-4.8972720
H	-0.5687600	-4.1149250	-6.0544600
C	-4.2035450	5.2045950	2.5635460
H	-5.1767210	5.5927200	2.2030880
H	-3.9625010	5.6798470	3.5264930
H	-3.4224660	5.5142660	1.8346470
C	-4.9131820	3.2138460	3.9006790
H	-4.9476280	2.1017850	3.8808530
H	-4.3828680	3.5282490	4.8133860
H	-5.9558540	3.5748390	3.9591300
C	1.0716990	-0.3703230	-1.0432840
H	1.3125150	0.4990820	-0.3984240
H	1.2383240	-1.3023710	-0.4646640
H	1.7980240	-0.3870980	-1.8842260
C	-0.5375990	0.7475950	-2.5777790
H	0.2286470	0.6766820	-3.3734430
H	-1.5358240	0.6360620	-3.0482130
H	-0.4742500	1.7561130	-2.1256310
C	2.9716980	-5.5628870	1.7618500
H	2.5236670	-6.1871820	0.9602240
H	3.9668890	-5.9561650	2.0141530
H	2.3168040	-5.6648170	2.6527780
C	4.1079990	-3.8477590	0.3478830
H	4.1025880	-2.7713790	0.0459570
H	5.1052180	-4.0658720	0.7633300

H	3.9763810	-4.4450060	-0.5718090
C	3.8461920	5.1600340	-0.3860210
H	4.6058030	4.5643610	0.1901930
H	4.4121070	5.7738960	-1.1046250
H	3.3514870	5.8314610	0.3359050
C	1.8580970	5.0166150	-1.8762950
H	2.3255960	5.8315620	-2.4524390
H	1.3764650	4.3374260	-2.6097790
H	1.0738880	5.4435230	-1.2218850
C	-4.3446820	-3.8474410	0.9198680
H	-4.5994900	-4.8956460	0.7039270
H	-5.2220400	-3.3322070	1.3499140
H	-4.1456880	-3.3467600	-0.0617600
C	-3.3109390	-4.5696330	3.0479040
H	-3.4107030	-5.6395640	2.7963410
H	-2.4254260	-4.4706640	3.7158340
H	-4.1991360	-4.2705710	3.6301730

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>7</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>6</sub>]<sup>+</sup>**

S	0.2238520	-2.8042000	-2.0407150
O	1.6651810	-3.0412410	-1.8283350
O	-0.6836010	-3.3752390	-1.0231480
O	-0.1407710	-3.7887270	-3.3785120
O	-0.1352620	-1.4559910	-2.4696230
H	0.6150850	-4.1813980	-3.8314290
H	-1.1107760	0.0971800	-2.2035200
N	-1.0350550	0.9514130	-1.5900910
H	-1.4710640	0.6827970	-0.6550080
C	-1.7967730	2.0952890	-2.1980780
H	-1.8078670	2.9755000	-1.5175410
H	-1.3702500	2.4086700	-3.1615930
H	-2.8544600	1.7965350	-2.3529330
C	0.4122270	1.2935040	-1.3885090
H	0.5433700	2.1006210	-0.6285560
H	0.9657180	0.4057030	-1.0188920
H	0.9053870	1.6241520	-2.3178940
S	3.9477910	1.9509120	-0.9910310
O	5.0304060	1.1216630	-1.5450530
O	3.0172250	1.2070710	-0.1414320
O	3.0576320	2.3180050	-2.4155740
O	4.2598130	3.3005610	-0.5093160
H	3.4268940	1.9391450	-3.2240390
N	0.0396350	-3.1985710	3.0364480
C	0.6889040	-3.9268120	4.1793750
H	1.7031170	-4.3124340	3.8894990

H	0.8453660	-3.2486460	5.0351600
H	0.0933020	-4.7859560	4.5231510
C	-0.3809570	-4.1316210	1.9369550
H	-1.0518750	-4.9234020	2.2929500
H	-0.9068590	-3.5618130	1.1294700
H	0.5008150	-4.6037850	1.4445740
H	0.7323440	-2.4783370	2.6325180
H	-0.7980140	-2.6423140	3.3829520
N	5.3187520	-1.5410280	-1.3062220
H	4.7398950	-1.4285840	-0.4106420
H	5.3204950	-0.6031590	-1.8015540
C	4.6757830	-2.5937380	-2.1632390
H	4.7230760	-3.5888600	-1.6773950
H	3.5849780	-2.3864960	-2.2902150
H	5.1404520	-2.6659830	-3.1564820
C	6.7221600	-1.9180820	-0.9138990
H	7.2324650	-1.0539100	-0.4489250
H	6.7009590	-2.7318880	-0.1565760
H	7.3238260	-2.2518800	-1.7731920
N	2.5733850	5.3404300	-0.8117610
H	1.8313530	4.6651560	-0.4091140
C	2.3990960	5.4136570	-2.3032250
H	3.1674410	6.0446240	-2.7797660
H	2.4894740	4.3871490	-2.7329230
H	1.4067580	5.8102050	-2.5784900
C	2.4220010	6.6832850	-0.1560980
H	1.3458430	6.9870340	-0.1043480
H	2.7891300	6.6512000	0.8850430
H	2.9725620	7.4782700	-0.6840640
H	3.5257900	4.9134370	-0.5921620
S	-0.8187830	4.7902490	0.6095610
O	0.3321400	4.0249800	0.0491970
O	-0.6013720	6.2244690	0.5606690
O	-0.7561840	4.4187690	2.2652160
O	-2.1144750	4.2333890	0.1876170
H	-0.7441170	5.1828960	2.8591450
S	3.2225120	-3.0170170	1.6445160
O	3.4182970	-3.7933320	2.8538100
O	2.2193800	-1.9131910	1.8633400
O	2.4073370	-4.0579940	0.6208540
O	4.3949690	-2.5559040	0.8788330
H	2.2785160	-3.7496300	-0.3262530
H	0.7556680	0.0542000	1.6299680
N	1.5418130	0.5749460	2.1224590
H	2.4222970	0.2749910	1.6273550
C	1.3381270	2.0553800	1.9795080

H	0.4313650	2.4108500	2.5035460
H	2.2028110	2.6275540	2.3456130
H	1.2082790	2.3172650	0.8956150
C	1.5875470	0.1739990	3.5729440
H	2.0616850	-0.8262510	3.6698380
H	2.1625750	0.8832490	4.1856750
H	0.5601240	0.0926890	3.9912520
S	-1.9733550	-0.4759940	2.0112950
O	-1.2492640	-0.8909850	3.2339970
O	-3.1397550	0.4038870	2.1306950
O	-2.5467070	-1.9466650	1.4723710
O	-1.0007550	0.0078020	0.9932360
H	-3.4169110	-1.9277920	0.9579390
H	-3.8364940	1.6075720	0.6922950
N	-4.2262020	2.5754160	0.9161670
H	-3.3935210	3.2364230	0.9401320
C	-5.1797230	3.0054440	-0.1646820
H	-4.6320850	3.1481500	-1.1145690
H	-5.9618570	2.2319610	-0.3458160
H	-5.6818620	3.9550010	0.0810160
C	-4.8980810	2.5405410	2.2615870
H	-5.8365670	1.9571410	2.2335870
H	-4.2354580	2.0177330	2.9921780
H	-5.1224290	3.5496840	2.6371320
S	-4.8115430	-0.5353610	-1.0673900
O	-3.6916990	0.4205810	-0.9598060
O	-4.5013410	-1.8219710	-0.3770390
O	-4.7934320	-1.0651550	-2.6834980
O	-6.1149720	0.0626340	-0.8881060
H	-5.5617500	-0.8040920	-3.2128010
N	-3.2913410	-3.9224280	-1.5065320
H	-4.0993490	-3.3577610	-1.0939600
C	-3.3024420	-3.7981220	-3.0044060
H	-2.3221800	-4.0899850	-3.4430020
H	-4.0856130	-4.4125000	-3.4744100
H	-3.4949180	-2.7396000	-3.2936090
C	-3.3750580	-5.3546890	-1.0600220
H	-2.5022590	-5.9353580	-1.4166040
H	-3.3773520	-5.4097770	0.0446500
H	-4.2890090	-5.8518170	-1.4272040
H	-2.3779780	-3.4875150	-1.1222110

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>7</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>7</sub>]<sup>+</sup>**

S	0.0477700	4.9902830	0.9024360
O	0.3653530	6.3784430	1.1034900

O	1.1692560	4.0303310	0.7703430
O	-0.5110210	4.9899180	-0.7462230
O	-1.0934220	4.4301170	1.6487440
H	-0.6991950	5.8652200	-1.1013510
S	1.2211130	-2.8652670	1.9422290
O	2.6569280	-3.2429970	1.9348880
O	0.8381660	-1.6490290	2.6551260
O	0.6386700	-4.1030080	2.9893670
O	0.4106320	-3.2054230	0.7470860
H	1.3209160	-4.5739580	3.4786210
S	-3.8775360	-0.2792040	1.3039760
O	-3.7245570	-1.5737980	1.9716110
O	-4.9033710	-0.1526070	0.2562870
O	-2.3834190	-0.0142270	0.5138630
O	-3.8403320	0.8845930	2.2313290
H	-1.9753970	-0.8643700	0.1416320
S	2.6367720	-0.9007120	-0.8315410
O	2.1638310	-1.8829450	-1.7948190
O	2.3233920	-1.2107590	0.5841870
O	1.9434160	0.5567600	-1.1632270
O	4.1089850	-0.5866530	-0.9641130
H	0.9174910	0.6548080	-0.9552280
S	-2.7742420	-2.8012260	-1.7756650
O	-2.2212470	-4.1718110	-1.7475880
O	-3.9827360	-2.5442970	-2.5621080
O	-1.5351450	-1.9638200	-2.5081530
O	-2.8470150	-2.2362970	-0.3938840
H	-1.6688700	-0.9601020	-2.5966330
S	-1.7185390	1.5441940	-1.2006970
O	-2.6719760	2.3632050	-0.4502370
O	-0.5114100	1.0442560	-0.4587170
O	-0.9861880	2.6652680	-2.2257690
O	-2.3169470	0.5532030	-2.1242520
H	-0.9788370	3.5972570	-1.8687570
S	5.8964090	0.8737370	-0.9964770
O	6.0371310	0.2878700	0.3133350
O	4.9241480	1.8995420	-1.2639560
O	6.0576400	-0.2209010	-2.2162390
O	7.3744650	1.5464910	-1.3683960
H	5.3036380	-0.8867140	-2.3022580
H	7.8755970	1.1131820	-2.0896300
N	2.4731320	3.2228670	-1.4523810
C	1.8954700	3.2382720	-2.8391130
C	3.4603120	4.3393710	-1.2359920
H	1.1005740	2.4605120	-2.9260830
H	1.4157670	4.2038430	-3.0733280

H	2.6618100	3.0318700	-3.6038900
H	3.5954160	4.5051400	-0.1473770
H	4.4497990	4.0794190	-1.6617150
H	3.1187800	5.2912300	-1.6714240
H	1.6854780	3.3085830	-0.7310900
H	2.9528110	2.2919520	-1.2816710
N	-3.6633980	3.5528220	1.5425800
C	-4.8515890	3.8685610	0.6783720
C	-3.7295820	4.2486190	2.8729520
H	-4.7272050	3.3462610	-0.2954980
H	-5.7893070	3.5120520	1.1371640
H	-4.9444910	4.9474720	0.4790830
H	-2.7074290	4.3096850	3.3057430
H	-4.0919940	5.2861310	2.7872530
H	-4.3816700	3.7048880	3.5771410
H	-3.6093780	2.4817320	1.6830980
H	-2.7642210	3.8208900	1.0361740
N	-2.3646670	-3.8412690	1.6363460
C	-2.3363250	-3.7937940	3.1392570
C	-2.6198670	-5.2297270	1.1241010
H	-2.4794200	-2.7418030	3.4713220
H	-3.1529370	-4.3792100	3.5884810
H	-1.3680800	-4.1603630	3.5400120
H	-2.5505800	-5.2436100	0.0084090
H	-1.8801610	-5.9499280	1.5116390
H	-3.6254500	-5.5877900	1.3986170
H	-3.1178070	-3.1537250	1.2741890
H	-1.4446830	-3.4908490	1.2438950
N	4.8007750	-1.5813310	1.8757730
C	4.7946670	-0.5948400	3.0100770
C	5.9547150	-2.5380710	1.9780910
H	3.8491870	-0.0200300	2.9965430
H	4.8699430	-1.0920800	3.9908710
H	5.6301620	0.1258970	2.9121910
H	5.9051430	-3.2778220	1.1579950
H	6.9238330	-2.0106450	1.9018320
H	5.9353030	-3.0999760	2.9278590
H	3.8514800	-2.1330210	1.8548120
H	4.8718780	-1.0442120	0.9582100
N	-5.2480710	-0.1357860	-2.3063680
C	-6.7067540	-0.0113960	-1.9664750
C	-4.8968210	0.5329910	-3.6038520
H	-6.8573520	-0.3635810	-0.9180670
H	-7.0582840	1.0309830	-2.0101080
H	-7.3354560	-0.6224470	-2.6338760
H	-3.7848220	0.5500250	-3.7144020



H	-5.3114060	-0.0117840	-4.4684670
H	-5.2456420	1.5760290	-3.6459310
H	-4.6644190	0.2708240	-1.5109550
H	-4.9805830	-1.1759360	-2.3546800
N	0.5563940	-4.0898350	-1.8299300
C	0.7552880	-3.7755480	-3.2872420
C	1.4360250	-5.2181550	-1.3694310
H	0.0169140	-2.9981740	-3.5942610
H	1.7571800	-3.3349640	-3.4629060
H	0.6178160	-4.6577810	-3.9273780
H	1.3254670	-5.3477140	-0.2732950
H	1.1768770	-6.1683020	-1.8636770
H	2.5017080	-5.0039030	-1.5663210
H	0.7741650	-3.2214200	-1.2510140
H	-0.4682200	-4.3322690	-1.6531360
N	-0.2064350	0.8231800	2.3216330
C	1.2215780	1.2915240	2.2744150
C	-1.0497540	1.6923570	3.2060440
H	1.8361900	0.5098480	1.7720150
H	1.3153900	2.2418670	1.6987770
H	1.6349300	1.4560610	3.2790140
H	-2.1160330	1.3566040	3.1749300
H	-0.7156870	1.6693640	4.2531280
H	-1.0321950	2.7518340	2.8589730
H	-0.6109250	0.8195130	1.3276340
H	-0.2255660	-0.1783120	2.6623880

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>7</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>8</sub>]<sup>+</sup>**

S	0.1533190	0.5514500	2.8795000
O	1.5296520	0.9619390	2.7454600
O	-0.0353490	0.2828440	4.5466330
O	-0.3568010	-0.6888580	2.3563560
O	-0.8693770	1.8127220	2.9459290
H	-0.4527360	1.0028700	5.0463950
H	4.7362950	4.8039130	-2.6368130
S	5.2213760	3.0175770	-1.3225860
O	5.6590990	3.3166230	0.0310010
O	4.1778810	1.9103070	-1.2763300
O	6.2079750	2.7656960	-2.3605050
O	4.3488060	4.3464620	-1.8727970
O	4.5160710	-2.9763890	3.1418890
H	5.0215260	-3.8096460	3.1873820
S	3.5516480	-2.7686710	1.7802390
O	4.0467520	-1.5279270	1.2291400
O	2.2081440	-2.9270710	2.2618380

O	4.1899180	-4.1379880	1.1322060
H	3.8278420	-4.4006280	0.2229270
S	2.4870690	-2.5889290	-1.7183180
O	3.6878130	-2.7749170	-2.5554560
O	1.1988270	-2.9447400	-2.2914080
O	2.4965850	-0.9183320	-1.6332440
O	2.7264640	-3.0698560	-0.3175070
H	1.6021260	-0.4426420	-1.6687420
H	2.5591210	2.1607210	-1.0370840
O	-0.0756910	1.3442910	0.8074600
S	0.2937560	1.7778270	-0.5704170
O	0.3755790	0.7246060	-1.5903440
O	1.8453410	2.3164120	-0.3107330
O	-0.4518040	2.9978760	-0.9419340
S	-4.4928000	-0.5579490	-2.5134550
O	-4.5074500	0.8918500	-2.7840370
O	-5.7478980	-1.1359880	-2.0662630
O	-3.6476130	-1.3226950	-3.4411890
O	-3.5870180	-0.6471390	-1.0434730
H	-2.8340280	-1.2993190	-1.0549220
S	-2.4936700	-3.9630370	0.0505480
O	-1.5376640	-5.0415140	0.2049590
O	-2.8130280	-3.2321840	1.3110170
O	-3.9620210	-4.7321290	-0.2879480
O	-2.2964620	-3.0412270	-1.0849370
H	-3.9090090	-5.6835520	-0.4621360
H	-1.5270410	1.9559630	2.1086770
S	-4.0237440	3.0226160	1.3998510
O	-4.4671130	3.3553600	0.0472780
O	-2.5267420	3.0319610	1.5075200
O	-4.6975460	1.9460550	2.1002260
O	-4.3593080	4.4195010	2.3060100
H	-5.0631730	4.3398650	2.9623150
N	-0.4727510	-3.2293520	2.9784760
C	-0.0971020	-4.6725300	2.7904990
C	-0.5203540	-2.8671430	4.4378510
H	-0.2197070	-4.9743370	1.7177180
H	0.9654760	-4.8396880	3.0447690
H	-0.7255080	-5.3510660	3.3859260
H	-0.7161220	-1.7765980	4.5572490
H	-1.3094550	-3.4186110	4.9722230
H	0.4449720	-3.0702490	4.9359730
H	0.2401070	-2.6114870	2.4873190
H	-1.4135100	-3.0238160	2.5246010
N	-5.1566510	-1.7529030	0.9922370
C	-5.7920790	-0.7749830	1.9358860

C	-6.1722510	-2.6760200	0.3765180
H	-5.0483900	-0.0139710	2.2814680
H	-6.5913040	-0.1908880	1.4422120
H	-6.2200860	-1.2648340	2.8221840
H	-5.6722110	-3.5686750	-0.0622550
H	-6.9243540	-3.0237670	1.0966850
H	-6.6911810	-2.1742350	-0.4768090
H	-4.6522560	-1.2153700	0.2051980
H	-4.4085140	-2.3160740	1.4922700
N	3.9771250	1.2967260	1.5571740
C	5.3830110	0.9356230	1.9515970
C	3.6110020	2.6602780	2.0805960
H	5.6225600	-0.0910610	1.6082880
H	6.1088790	1.6519440	1.5062630
H	5.5198380	0.9565490	3.0454890
H	2.6188200	2.9509490	1.6619050
H	3.5263650	2.6600940	3.1781530
H	4.3622020	3.4175990	1.7621960
H	3.8869830	1.2968970	0.4968650
H	3.2985560	0.5781180	1.9181560
N	-0.5765680	4.5326900	1.3801170
C	-1.3968800	5.7488370	1.7095690
C	0.8824950	4.8663520	1.2621440
H	-2.4542360	5.4485860	1.9178490
H	-1.0306720	6.2674990	2.6109940
H	-1.4093400	6.4716820	0.8781070
H	1.4912630	3.9350510	1.1118170
H	1.0853860	5.5005900	0.3786730
H	1.2683950	5.3847020	2.1537710
H	-0.7309490	3.7918890	2.1208300
H	-0.9293760	4.0788210	0.4663250
N	-4.0877150	3.2500370	-2.5490190
C	-2.9211610	4.1737620	-2.3573650
C	-5.3757030	3.9982010	-2.7595300
H	-1.9966260	3.5910680	-2.1084140
H	-2.7153920	4.7820470	-3.2489600
H	-3.0929200	4.8442100	-1.4947100
H	-6.1860090	3.2811160	-3.0015990
H	-5.6736870	4.5165930	-1.8239830
H	-5.3074180	4.7371680	-3.5709540
H	-3.9154690	2.5944570	-3.3518470
H	-4.2001180	2.6275520	-1.6871800
N	-1.2268660	-2.5202800	-3.3301190
C	-0.7139770	-1.2007000	-3.8383200
C	-0.9745640	-3.6319600	-4.3109150
H	-0.6565930	-0.4634030	-3.0040900

H	0.3015400	-1.2889290	-4.2554530
H	-1.3963140	-0.7837370	-4.6004180
H	-1.4583530	-4.5626240	-3.9640720
H	-1.3723810	-3.3930830	-5.3110440
H	0.1117370	-3.8372040	-4.3946390
H	-0.7528150	-2.7570280	-2.4121000
H	-2.2758120	-2.4381430	-3.1328050
N	5.1197540	-0.4426580	-2.4994380
C	6.0293830	-0.7923320	-1.3530450
C	5.8820050	0.0963790	-3.6751210
H	5.4178230	-1.0601380	-0.4600180
H	6.6630580	-1.6639750	-1.5928840
H	6.6915050	0.0478250	-1.0827730
H	5.2025320	0.2857410	-4.5232060
H	6.3744170	1.0746030	-3.4317530
H	6.6674780	-0.5983460	-4.0132020
H	4.5770240	-1.3281820	-2.7899650
H	4.4025810	0.2776630	-2.1628570



S	0.8656750	3.6493160	2.2038740
O	2.3198060	3.6495260	2.3069020
O	0.2181210	4.9457850	1.9606070
O	0.2950440	3.0862800	3.6512070
O	0.3028540	2.6097560	1.2286860
H	0.9268360	2.4471550	4.1282740
N	-2.2381590	-0.1884080	2.4626200
H	-3.1851960	-0.6476750	2.6941300
H	-1.4905260	-0.7166270	2.9753460
C	-1.9796750	-0.2791650	0.9851580
H	-2.5949510	0.4393120	0.4070160
H	-0.9117670	-0.0640160	0.7519680
H	-2.2040800	-1.2918520	0.5918640
C	-2.2442330	1.2363090	2.9438670
H	-1.2428690	1.7101420	2.8369970
H	-2.9498100	1.8588300	2.3604280
H	-2.5213560	1.2864040	4.0100970
S	1.3296800	-0.3611390	3.5065790
O	1.8502910	0.9641430	3.8595010
O	0.6991220	-0.4243400	2.1790650
O	-0.0524140	-0.5960910	4.4763580
O	2.1902990	-1.4946760	3.8696950
H	0.0827330	-1.0548130	5.3141160
N	3.7102740	-3.4322570	2.7958730
H	2.7965160	-2.9738520	3.1015360

C	4.8518980	-2.4972730	3.0838150
H	5.8276820	-2.9396520	2.8304080
H	4.7359090	-1.5605580	2.4864920
H	4.8570900	-2.1909070	4.1455160
C	3.8755180	-4.7475500	3.5050180
H	3.0353920	-5.4252970	3.2267970
H	4.8134530	-5.2541690	3.2243710
H	3.8623030	-4.6228290	4.6008800
H	3.6197270	-3.5915440	1.7513950
S	1.2408040	-5.1867960	0.2164010
O	-0.1866610	-5.1730450	0.1263060
O	1.8784350	-4.3179270	-0.9796250
O	1.9184850	-4.9082130	1.4586280
H	2.6452790	-3.5692800	-0.7114400
O	1.7809320	-6.6615330	-0.3240930
H	2.1865050	-6.6696310	-1.2141130
S	4.2432860	-1.4676730	-0.4418270
O	3.4871610	-2.6795750	0.0713190
O	3.6520860	-0.8979390	-1.6735210
O	5.6912740	-2.1408630	-0.8268960
O	4.4693240	-0.5097190	0.6422410
H	6.1911310	-1.7231160	-1.5971960
H	2.2236310	-1.2345530	-3.0413780
N	1.1801720	-1.0334110	-3.0834880
C	0.4824840	-1.7387280	-1.9573430
H	0.7549680	-1.2715450	-0.9858200
H	-0.6225740	-1.6777150	-2.0474220
H	0.7456340	-2.8119200	-1.9205550
C	0.6398080	-1.4363570	-4.4266490
H	-0.4434410	-1.1770830	-4.5198890
H	1.1990630	-0.9187960	-5.2283250
H	0.7314250	-2.5205140	-4.5963840
H	1.0830970	0.0144080	-2.9591700
S	-3.2894950	-1.1978010	-2.5615100
O	-2.2314680	-0.9896860	-3.5437470
O	-4.6293840	-1.5778480	-3.0004110
O	-3.5265800	0.3748360	-1.9393600
O	-2.8404700	-1.9727450	-1.3723220
H	-3.0225450	1.0815980	-2.4249630
H	-3.7625230	-3.2511520	-0.6700400
N	-4.1686070	-4.2518410	-0.6592290
H	-4.4736030	-4.4270670	0.3310180
C	-3.1113400	-5.2351240	-1.0667110
H	-2.1938440	-5.1073540	-0.4411180
H	-3.4459740	-6.2787100	-0.9601580
H	-2.7928060	-5.0785980	-2.1118440

C	-5.3738000	-4.2903240	-1.5603610
H	-5.6748530	-5.3121250	-1.8281930
H	-6.2255960	-3.7964610	-1.0414120
H	-5.1999000	-3.7057230	-2.4910760
S	-5.6740230	-1.7097890	1.8093990
O	-5.4229200	-2.8858550	0.9655660
O	-4.6224900	-1.4666770	2.8264130
O	-7.0077780	-2.0850230	2.7512650
O	-6.0381150	-0.5085330	1.0406360
H	-6.8485570	-2.0683650	3.7101280
H	3.4436640	2.9295910	1.0918150
N	4.2309930	2.1959850	1.1953080
H	3.8223540	1.2582340	0.9446920
C	5.3470750	2.5042700	0.2375180
H	4.9502560	2.5204620	-0.8038530
H	5.8032890	3.4850200	0.4435030
H	6.1364870	1.7320360	0.2730580
C	4.6870520	2.1598760	2.6278130
H	5.1243870	3.1223920	2.9396930
H	3.7957990	1.9972210	3.2874950
H	5.4112960	1.3518410	2.8072240
S	1.0876410	2.1876460	-0.9465500
O	2.1110270	3.0117100	-0.3028820
O	-0.2550860	2.8425150	-1.1266410
O	0.8931290	0.7488430	-0.1817520
O	1.5667990	1.6608840	-2.2883660
H	0.6594180	0.7597560	0.8306370
N	-0.5010530	6.4071600	-0.0790300
H	-0.7220110	5.5799620	0.5693450
H	-1.3797830	6.6158360	-0.6050740
C	0.5724930	5.9810090	-1.0421380
H	0.8584200	6.7823100	-1.7387730
H	1.4810760	5.6358480	-0.5056640
H	0.2063940	5.1085160	-1.6304090
C	-0.0824040	7.5830350	0.7585210
H	-0.9391360	7.9738840	1.3372110
H	0.6758390	7.2605320	1.5092530
H	0.3417900	8.4029960	0.1595160
H	-6.1267120	0.0608400	-0.6108280
N	-6.1017490	0.9784700	-1.1542430
C	-6.6413920	0.7599600	-2.5383880
H	-6.5333560	1.6580640	-3.1681590
H	-6.0773940	-0.0736480	-3.0349780
H	-7.7041840	0.4696400	-2.5268530
C	-6.8665070	2.0255580	-0.3890100
H	-6.7344940	1.8447150	0.6996620

H	-6.4747620	3.0390160	-0.6121320
H	-7.9455970	2.0000840	-0.6004550
H	-5.0843500	1.2706340	-1.2122590
S	-2.8072080	3.4910710	-0.8655560
O	-2.2767250	4.8411270	-0.8263800
O	-2.2070580	2.6507120	0.3627060
O	-4.2350500	3.2672920	-0.8493290
H	-1.1367360	2.7118570	0.5436800
O	-2.3330520	2.7496500	-2.2592350
H	-1.3127530	2.6730160	-2.3933320
S	4.6928690	0.2357780	-3.4505420
O	5.7458860	-0.3782630	-2.6695980
O	4.1324530	1.5466140	-2.6828230
O	3.6433560	-0.4994680	-4.1048750
H	3.0584590	1.6023830	-2.5225260
O	5.4743970	1.1078280	-4.6365530
H	5.4978900	2.0741060	-4.5049300

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>7</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>10</sub>]<sup>+</sup>**

S	1.3429140	1.9131340	-2.0879220
O	-0.0390970	1.9925360	-1.6672860
O	2.1484200	3.1538910	-1.9135350
O	1.2253350	1.8852580	-3.8215570
O	2.0660010	0.6242510	-1.9444980
H	1.6349030	2.6335700	-4.2696050
N	2.3955320	-0.7393430	-4.4070340
H	2.7009230	-0.9383890	-3.3983840
H	1.7616330	0.1040570	-4.3452210
C	3.5945420	-0.3988480	-5.2492620
H	3.3093110	-0.0014150	-6.2349140
H	4.2286050	0.3639880	-4.7256800
H	4.2506140	-1.2723090	-5.4073470
C	1.6527670	-1.9142670	-4.9672580
H	0.7385290	-2.1568690	-4.3548700
H	1.2864170	-1.7351890	-5.9916470
H	2.2650010	-2.8303900	-4.9815590
S	-2.0170670	-1.9505330	-3.0297700
O	-2.1747220	-0.5096140	-3.2187150
O	-1.0165220	-2.5847580	-3.8696990
O	-3.4946060	-2.6350690	-3.3406260
O	-1.8280250	-2.3421160	-1.5574680
H	-4.2888220	-2.0261690	-3.1544280
N	-2.7942010	2.0681300	-2.9251520
H	-3.0960980	1.0692050	-2.6801790
H	-2.2388740	2.3989960	-2.0897570

C	-4.0127960	2.9307030	-3.1125800
H	-3.7537790	3.9915550	-3.2425450
H	-4.6196850	2.5989680	-3.9700700
H	-4.6549350	2.8506180	-2.2020910
C	-1.9364960	2.0585800	-4.1590560
H	-1.0059430	1.4801310	-3.9553530
H	-2.4435670	1.5386850	-4.9907780
H	-1.6575380	3.0706190	-4.4805540
S	2.6494150	-2.8092790	-0.0677530
O	3.9480570	-2.3397250	0.3880900
O	2.8462960	-3.5798360	-1.5017610
O	2.0204590	-3.8021610	0.8238330
H	3.3518490	-3.0521130	-2.1886410
O	1.5989780	-1.6018670	-0.2614990
H	1.8646000	-0.8719240	-0.9772010
S	-4.9849420	-0.3424910	-0.6392550
O	-4.9877860	-1.4315620	-1.6652150
O	-4.4140090	-0.8729920	0.6208070
O	-6.5867610	-0.0078820	-0.4586520
O	-4.3146230	0.8827510	-1.1501040
H	-6.7912590	0.7411240	0.1666180
H	-2.8143590	-0.5164610	1.1749010
N	-1.8847060	-0.2152780	1.6114500
H	-2.0121640	0.7937460	1.9163180
C	-1.6141570	-1.0625700	2.8211700
H	-2.4738470	-1.0017210	3.5167090
H	-1.4378060	-2.1226540	2.5599220
H	-0.7126040	-0.7155300	3.3784400
C	-0.7864120	-0.2866310	0.5932380
H	-0.7799840	-1.2548930	0.0505970
H	-0.9029900	0.5169450	-0.1639640
H	0.2194700	-0.1713890	1.0521350
H	1.1924670	1.7672670	2.1683670
S	2.1585530	0.3965030	3.7506740
O	2.1575110	1.6112680	4.5143220
O	3.4658120	-0.2429250	3.4529790
O	1.6617580	0.9154770	2.1855720
O	1.1452180	-0.6403310	4.0652420
H	1.2411160	-2.3148840	3.9579210
N	1.6472910	-3.2965480	3.7595080
H	1.4351620	-3.5096960	2.7348290
C	0.9553000	-4.3140320	4.6232410
H	1.4161590	-5.3124990	4.5394560
H	0.9572330	-4.0172790	5.6854540
H	-0.1020810	-4.4128550	4.2909930
C	3.1318370	-3.2731110	3.9854860



H	3.5655900	-2.3385620	3.5447730
H	3.3878080	-3.2572780	5.0581340
H	3.6314720	-4.1368320	3.5191320
S	4.4870310	-0.1412640	-1.5353110
O	3.4661110	-1.2791570	-1.7179320
O	4.8328010	0.4344550	-2.8146780
O	5.7989740	-1.0200190	-0.9844770
O	4.2014250	0.7617280	-0.3937750
H	5.5412070	-1.8484790	-0.4951240
H	3.9322510	3.3187760	-1.9570310
S	3.6296610	3.0744180	0.2673080
O	4.5181580	2.5893090	1.2935860
O	2.9751350	4.3587380	0.4338230
O	2.3211560	2.0497730	0.1322240
O	4.4676100	3.1117960	-1.1272250
H	2.4981860	1.0963950	0.4817400
H	-3.8598420	2.2260140	-0.3032260
S	-2.7514820	3.7219260	1.0632870
O	-1.6829700	4.6488910	0.6737010
O	-2.3028010	2.5828550	1.9289950
O	-3.1534800	2.9861040	-0.3703300
O	-4.0041340	4.2843350	1.5832240
H	1.5603170	4.9610000	-0.6421820
H	0.0638130	4.5053190	0.0576770
N	0.6384110	5.3344190	-0.2741900
C	-0.1250800	6.0379070	-1.3628590
H	-1.1562890	6.2690900	-1.0120630
H	0.3578210	6.9806830	-1.6662580
H	-0.2166980	5.3893690	-2.2495820
C	0.8856330	6.2407580	0.9035570
H	1.6287500	5.7674060	1.5831640
H	1.2958800	7.2169880	0.6031800
H	-0.0530300	6.4034430	1.4704530
H	4.8734960	0.4852760	2.7768530
H	5.3366920	0.7529150	1.1600420
N	5.7149050	0.4492220	2.1111400
C	6.2351980	-0.9570400	2.0344860
H	6.9906050	-1.0673040	1.2349010
H	6.6787100	-1.2855300	2.9871910
H	5.3916400	-1.6482560	1.7973970
C	6.7695550	1.4183140	2.5662570
H	7.6561580	1.4015330	1.9108250
H	6.3521910	2.4516360	2.5309510
H	7.0937260	1.2178960	3.6000490
S	-5.3738170	1.3196940	2.7105720
O	-5.3873880	1.3054720	1.2408770

O	-6.2455730	0.4755650	3.4432290
O	-5.5309090	2.8637520	3.1687590
O	-3.8240800	1.0564930	3.1843510
H	-5.1708970	3.6132570	2.5379500
H	-3.1868800	1.8742820	3.1418660
S	-0.4525250	-4.4593790	0.6837930
O	-1.7915620	-4.8701380	0.3262440
O	0.5303190	-5.7633720	0.5341400
O	-0.2771550	-3.8851340	2.0105840
H	1.5072230	-5.5513970	0.4648500
O	0.1253090	-3.4733750	-0.4401580
H	-0.6167120	-2.9604430	-1.1007750
H	-4.7560150	-3.1251220	-1.2575460
N	-4.1535990	-3.8427560	-0.7414130
H	-3.1608680	-3.4620970	-0.7535530
C	-4.1726360	-5.1575430	-1.4699840
H	-5.1585720	-5.6452940	-1.4236860
H	-3.9164870	-4.9945960	-2.5373190
H	-3.4172290	-5.8505590	-1.0415450
C	-4.6145540	-3.9704310	0.6829960
H	-3.9264520	-4.6168710	1.2627470
H	-4.6265590	-2.9616260	1.1623570
H	-5.6312460	-4.3865900	0.7558880

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>7</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>11</sub>]<sup>+</sup>**

S	-1.3951130	-0.9574500	3.8252740
O	0.0768190	-0.8307890	4.0447260
O	-2.1906440	0.0680330	4.4739520
O	-1.8383370	-2.3921530	4.4786870
O	-1.6913130	-1.1179200	2.3485390
H	-1.8261130	-3.2044400	3.8582570
N	-4.3520680	-0.3853220	1.5800610
H	-4.5629290	-0.2268430	0.5509500
H	-3.4295170	-0.9217390	1.6137920
C	-5.4322910	-1.2206940	2.2075140
H	-5.3209780	-2.2845650	1.8890330
H	-5.3638180	-1.2211720	3.3106860
H	-6.4369840	-0.8669600	1.9264730
C	-4.1955490	0.9400590	2.2706610
H	-3.8726000	0.8196880	3.3315150
H	-3.4007500	1.5370890	1.7763290
H	-5.1263100	1.5280050	2.2517410
S	-2.6404940	-4.5241840	1.4681730
O	-1.7028800	-4.2748570	2.5810260
O	-3.8346920	-3.6691350	1.3767270

O	-3.2254410	-6.0555210	1.8026420
O	-1.9896560	-4.6485750	0.1404690
H	-2.8400270	-6.4953010	2.5792010
H	1.2839850	-1.7699030	3.1559140
N	1.7620230	-2.4474940	2.4856860
H	2.8270490	-2.3139040	2.5680350
C	1.3474510	-2.1320980	1.0766420
H	0.2786350	-2.3462190	0.8880840
H	1.5134680	-1.0553210	0.8577820
H	1.9403420	-2.7124400	0.3371000
C	1.4097040	-3.8581950	2.8669320
H	1.7101680	-4.0648540	3.9088080
H	0.3130430	-4.0487740	2.7904370
H	1.9143000	-4.5925980	2.2157390
N	-4.3351710	-3.1982570	-1.3818790
H	-3.5001220	-2.7790140	-1.8773970
H	-4.1365100	-3.0822570	-0.3349290
C	-5.5801090	-2.4393140	-1.7400170
H	-5.7401220	-2.3925220	-2.8308560
H	-6.4805120	-2.8802270	-1.2816470
H	-5.4990400	-1.3872470	-1.3728550
C	-4.4370770	-4.6574450	-1.7282170
H	-3.4800700	-5.1648710	-1.4573230
H	-5.2474300	-5.1580290	-1.1721070
H	-4.5988000	-4.8135870	-2.8075050
S	-5.3586610	1.5052180	-2.0500070
O	-5.5773040	0.6989600	-0.8723920
O	-5.4634810	2.9523650	-2.0784190
O	-6.5675970	1.0214510	-3.0987480
O	-4.1518790	0.9251530	-2.9630290
H	-6.9335210	1.7183510	-3.6745060
S	5.0808340	-2.9070070	0.8184310
O	6.0918340	-3.9237190	0.8845500
O	4.0859740	-2.9963180	-0.2759730
O	5.9907350	-1.4982720	0.3202880
O	4.4468430	-2.4567670	2.0696410
H	6.9690690	-1.5995470	0.4070490
H	4.1898620	-2.3025800	-2.0511040
N	3.3700400	-2.5813260	-2.6788400
H	2.5028730	-2.2590490	-2.1883690
C	3.4677390	-1.8877950	-4.0098630
H	3.7108850	-0.8154470	-3.8418440
H	4.2756690	-2.3052380	-4.6322240
H	2.5120370	-1.9590940	-4.5599620
C	3.3293660	-4.0780460	-2.8247340
H	2.4279800	-4.4119060	-3.3734240

H	4.2200840	-4.4625710	-3.3479150
H	3.3203480	-4.5395190	-1.8115710
H	3.0776380	3.2055070	0.1630150
S	2.8050270	2.1125580	-2.3304630
O	3.5040550	0.9918060	-1.6527950
O	2.5461280	3.2306780	-1.3595600
O	1.6197560	1.7679420	-3.1108000
O	3.8512050	2.7080990	-3.4656660
H	4.8150610	2.5113030	-3.3142280
H	-0.2443100	1.1793010	-3.1796040
N	-0.6929220	1.1098810	-4.1415290
H	-1.6498570	0.7122690	-3.9928070
C	0.1269170	0.1749470	-4.9864890
H	-0.3081280	0.0190890	-5.9834690
H	1.1597120	0.5650410	-5.0987400
H	0.2227980	-0.8130090	-4.4743940
C	-0.7882640	2.4855180	-4.7373670
H	-1.3714880	3.1547330	-4.0560690
H	0.2191190	2.9376660	-4.8326460
H	-1.2721130	2.4844950	-5.7243370
S	-2.7242870	3.5331870	-1.0411630
O	-1.9309070	3.8923060	-2.2091230
O	-3.4140710	2.2133860	-1.1184560
O	-3.9160020	4.6495870	-0.8194940
O	-1.9410190	3.6773460	0.2360940
H	-4.8006070	4.4370390	-1.2551770
H	-2.8111490	4.5269110	1.6248980
S	-0.9489900	3.6252070	2.5181250
O	-0.0721500	4.3951480	1.6670250
O	-0.5778360	3.4150810	3.8972850
O	-1.1900030	2.1206880	1.9224880
O	-2.4490620	4.2784380	2.5324540
H	-1.2332890	2.0348950	0.9066090
H	3.1645410	0.5791040	0.0084970
S	3.2517770	1.7921930	1.9800790
O	2.3052690	1.8615240	3.0764940
O	3.2177840	3.2195200	1.2003790
O	2.5858250	0.8163850	0.8571990
O	4.5981360	1.4026960	2.2919830
H	0.8827910	2.3540590	4.5576090
H	0.8230210	0.6646100	4.7239580
N	0.8987270	1.5741910	5.2773700
C	2.2022210	1.6045310	6.0259210
H	3.0455100	1.5647630	5.3034030
H	2.3147340	2.5293500	6.6171460
H	2.3006930	0.7459380	6.7113890

C	-0.2815160	1.7163140	6.1971160
H	-0.3293660	2.7215910	6.6474950
H	-1.2304270	1.5885590	5.6119640
H	-0.2838080	0.9583860	6.9947580
H	-0.0981750	4.8438270	-0.1039520
N	0.7088180	5.1624560	-0.7263410
H	1.1489040	4.2827880	-1.1358200
C	0.1903910	6.0302790	-1.8363440
H	-0.5943710	5.4787300	-2.4115890
H	-0.2740070	6.9553890	-1.4552870
H	0.9885580	6.3156260	-2.5416030
C	1.7379010	5.8668280	0.1168870
H	1.3492490	6.8026590	0.5477340
H	2.0170810	5.2057500	0.9755480
H	2.6558830	6.0797310	-0.4542810
S	5.8143050	0.2709800	-1.2313710
O	5.2159940	-0.6248550	-2.1796770
O	7.2031970	0.1971970	-0.8820390
O	4.9475290	0.6112680	0.1297470
O	5.7066860	1.8378930	-1.9056380
H	5.3687360	0.2547370	1.0070170
H	6.4852850	2.3971910	-1.7076120
S	-0.3718590	-3.3705100	-2.6103380
O	-1.7959830	-3.1817660	-2.7801400
O	0.0203610	-4.7678560	-3.4675740
O	0.5997120	-2.4409890	-3.1519640
H	-0.1091100	-5.6070250	-2.9915210
O	0.0853660	-4.0431930	-1.2099790
H	-0.6140890	-4.0082430	-0.4264870
S	-1.6997000	-0.6895170	-0.9030730
O	-3.0421640	-1.1530300	-0.4987220
O	-0.7417270	-1.8184670	-1.0623480
O	-1.1164390	0.2646420	0.2890160
H	-1.1251880	-0.1507990	1.2675920
O	-1.7404830	0.2145100	-2.0908160
H	-3.2114180	0.8602380	-2.4671010

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>7</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>12</sub>]<sup>+</sup>**

S	-2.8809790	-3.1437070	0.1538480
O	-1.7829480	-4.0850260	0.4833100
O	-3.2654320	-2.3331120	1.3168390
O	-4.2113850	-4.0713200	-0.1405640
O	-2.6532570	-2.3641930	-1.1017550
H	-4.3576030	-4.3249300	-1.1167930
N	-4.7654760	-0.0640330	-1.0821120

H	-4.2348960	0.8359150	-0.8784160
H	-4.0560130	-0.7725440	-1.4556210
C	-5.7970320	0.2148860	-2.1474340
H	-5.4212760	-0.1444720	-3.1287030
H	-6.7554160	-0.2904170	-1.9571230
H	-5.9789700	1.3062760	-2.2248490
C	-5.3933480	-0.5687360	0.1851070
H	-5.9062620	-1.5355260	0.0381560
H	-4.6113210	-0.7397230	0.9663900
H	-6.1176480	0.1511830	0.6003990
S	-3.0785630	-2.7642110	-3.3330510
O	-3.7848220	-3.8722740	-2.6810260
O	-3.6538300	-1.3986900	-3.2041100
O	-3.3881740	-3.0857050	-4.9731170
O	-1.5874370	-2.7965890	-3.3161190
H	-3.9220150	-3.8747960	-5.1446870
H	-0.3499000	-4.4670420	-0.4522530
N	0.7046770	-4.6191430	-0.4418660
H	1.1421430	-3.6611510	-0.2707420
C	1.1690360	-5.1685330	-1.7600020
H	0.6315260	-6.0908600	-2.0335770
H	1.0028810	-4.4253640	-2.5732360
H	2.2519480	-5.4050760	-1.7366500
C	1.0640790	-5.5414280	0.6916040
H	0.7348270	-5.0977750	1.6551990
H	0.5909640	-6.5285680	0.5827380
H	2.1668540	-5.6881530	0.7529110
N	-2.4998450	0.6215050	-4.7426960
H	-1.5376580	1.0054890	-4.5071800
H	-2.7196920	-0.0941320	-3.9791440
C	-3.5189350	1.7240230	-4.7102960
H	-3.2275100	2.5709620	-5.3533400
H	-4.5156190	1.3734270	-5.0190940
H	-3.6072260	2.1276610	-3.6700320
C	-2.4589180	-0.0823090	-6.0710260
H	-1.5693320	-0.7510000	-6.0992030
H	-3.3438440	-0.7322170	-6.2118550
H	-2.3909510	0.6184600	-6.9159850
S	-3.3437660	3.5386740	-0.9431080
O	-4.2328810	2.6296210	-1.6678540
O	-3.7996850	4.1076430	0.3420490
O	-3.2684640	4.9423860	-1.8916020
O	-1.8955460	3.1405350	-0.9361590
H	-4.0741240	5.4741970	-1.9194380
S	4.6781500	-3.6716650	-0.4601620
O	5.6701000	-3.7229970	-1.4902760

O	3.6963030	-2.4350890	-0.8096820
O	5.3459490	-2.9674160	0.8888980
O	3.9180410	-4.8300210	-0.0939560
H	6.2278780	-3.2804810	1.2407550
H	4.8755160	-0.3159230	-1.5466530
N	4.5072880	-0.4842130	-2.5277820
H	3.6432840	-1.0942430	-2.4307950
C	4.1174530	0.8230630	-3.1608920
H	3.5404310	1.4367240	-2.4291470
H	4.9914570	1.4120270	-3.4763170
H	3.4551300	0.6535180	-4.0318070
C	5.5438520	-1.2046090	-3.3439820
H	5.1773960	-1.4317380	-4.3592970
H	6.4768490	-0.6218680	-3.4278080
H	5.8154370	-2.1759170	-2.8631630
H	1.4277460	-0.0481380	2.0233900
S	2.4670740	2.2804390	0.5391490
O	2.5843080	1.4189280	-0.6435800
O	1.7166480	1.6901040	1.6604180
O	2.1586570	3.7251890	0.2651830
O	4.0357900	2.4211510	1.1282300
H	4.5232440	3.2492060	0.8056060
H	0.7228450	5.1286060	0.6297880
N	-0.2947040	5.1076360	0.3187520
H	-0.4811840	4.1217810	-0.0567650
C	-0.4988180	6.1007350	-0.7937590
H	-1.5276520	6.0437770	-1.2089680
H	-0.3019210	7.1339620	-0.4611050
H	0.1972570	5.8835880	-1.6302610
C	-1.1880750	5.3959840	1.4896030
H	-1.0797830	4.6003270	2.2673120
H	-0.9685210	6.3745640	1.9435000
H	-2.2643420	5.3794750	1.2023300
S	-3.2021510	2.0236950	2.1181440
O	-1.9578740	2.6636230	2.5502720
O	-3.2421060	1.7748810	0.6291040
O	-4.4847740	2.9824580	2.4676740
O	-3.5311170	0.7824760	2.8845700
H	-4.6643580	3.7303130	1.8051930
H	-4.7797950	0.5987560	4.1685790
S	-2.9776330	-0.5464220	4.9160180
O	-2.0844610	0.5894990	4.9616060
O	-2.8595060	-1.5675570	5.9203040
O	-2.7600260	-1.4017170	3.5303140
O	-4.5423070	-0.0786790	4.8783370
H	-3.0583940	-0.9993080	2.6423040

H	3.0220320	-2.1158190	-0.0176300
S	1.6566990	-2.3067230	2.3983140
O	0.6202820	-3.2182570	2.8884860
O	0.9987720	-0.7886130	2.5584400
O	1.8886980	-2.4972480	0.9205110
O	2.9136920	-2.2788360	3.1567520
H	-2.4440840	-3.1581660	3.1198970
H	-1.1358790	-4.1323310	2.6662360
N	-1.9379140	-4.0713980	3.3535990
C	-1.4059510	-4.0132740	4.7595430
H	-0.4746400	-3.4034690	4.7750600
H	-2.1295230	-3.5252350	5.4517560
H	-1.1526700	-5.0053720	5.1599170
C	-2.8769550	-5.2303230	3.1621930
H	-3.8007210	-5.1017390	3.7553940
H	-3.1720490	-5.3161720	2.0945790
H	-2.4168460	-6.1888310	3.4543100
H	-0.9211760	1.6873890	4.0211050
N	0.0952570	2.0157680	3.9870630
H	0.4153780	1.9024650	2.9852990
C	0.1493280	3.4707110	4.3637260
H	-0.5289300	4.0433060	3.6852180
H	-0.2026920	3.6351980	5.3973920
H	1.1679750	3.8823790	4.2729880
C	0.9376500	1.1653660	4.8950400
H	0.4964180	1.0986090	5.9055190
H	0.9906890	0.1289720	4.4871140
H	1.9722010	1.5366290	4.9749170
S	5.9238960	-0.5370760	1.3643340
O	5.9151020	-0.2193240	-0.0487300
O	6.8527310	-1.4901450	1.9028350
O	4.3881570	-0.8924330	1.7670420
O	6.0666540	0.8611070	2.2090590
H	4.2265430	-1.6396810	2.4950820
H	5.3339640	1.5336510	2.0521510
S	0.5672150	-1.5688180	-3.4400730
O	-0.4079920	-0.7515580	-4.1256470
O	0.6196600	-3.0622260	-4.1589630
O	1.9658830	-1.1851820	-3.3930640
H	-0.2900780	-3.4546940	-4.3557350
O	0.1590090	-2.0002360	-1.9171310
H	-0.8594730	-2.0561900	-1.7382130
S	-0.3303680	1.7627970	-1.8230970
O	-1.0181790	2.0926190	-3.0448330
O	0.5134220	2.7048820	-1.0837260
O	0.7028290	0.5322530	-2.2674050



H	1.5636890	0.4776960	-1.7136820
O	-1.1994370	0.8318200	-0.8286000
H	-1.8719350	1.3188700	-0.1916390
S	3.2294920	5.5496040	-0.5527220
O	2.3309890	6.1809540	0.3744840
O	3.9127610	6.7743460	-1.4414260
O	2.3746330	4.9117910	-1.8014260
O	4.3573270	4.7135900	-0.1937550
H	1.8007400	4.0930370	-1.5588350
H	4.8104220	6.5997410	-1.7872370

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>8</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>7</sub>]<sup>+</sup>**

S	2.7008060	-3.7545760	-0.5664570
O	4.0453390	-3.5969810	-1.1481150
O	2.6899750	-3.6946660	0.9046150
O	2.2637850	-5.3691560	-0.8632930
O	1.6239560	-3.0391540	-1.2615090
H	2.4405620	-5.9843380	-0.1396630
N	-0.8762780	-3.6045460	-2.1071020
H	-0.2996410	-3.2087850	-1.3141620
H	-1.8798480	-3.3299510	-1.9027100
C	-0.4153170	-2.9861360	-3.3985240
H	0.6913160	-3.0000820	-3.4597640
H	-0.8292450	-3.4986150	-4.2793240
H	-0.7470940	-1.9260900	-3.4330740
C	-0.7328670	-5.1017710	-2.1073730
H	0.3353590	-5.4005510	-2.0367010
H	-1.2560360	-5.5148580	-1.2159940
H	-1.1714520	-5.5646860	-3.0027430
S	0.7942200	3.6552840	-3.1565050
O	1.9270790	3.9049040	-2.2612310
O	0.8724460	4.0993250	-4.5342500
O	-0.4505760	4.6600200	-2.5275100
O	0.1523490	2.3216390	-2.9863080
H	-0.3760550	5.5923860	-2.7504540
H	-1.3133480	-0.4381120	-0.7243140
N	-0.5165480	0.1291190	-0.3149630
H	-0.3624510	-0.2401330	0.6591090
C	0.7182560	-0.0766880	-1.1451640
H	1.6303240	0.2762350	-0.6196710
H	0.8796610	-1.1550980	-1.3594320
H	0.6581910	0.4759780	-2.1075230
C	-0.9000160	1.5800790	-0.2396940
H	-1.8989480	1.6792010	0.2425810
H	-0.1773180	2.1565740	0.3633930

H	-0.9596170	2.0395620	-1.2471250
H	3.7762270	3.3375770	0.7494510
N	3.4726070	3.9705570	-0.0519620
H	3.0083160	3.3500800	-0.7729860
C	2.4886030	4.9992370	0.4293870
H	1.9663740	5.4664530	-0.4284410
H	1.7100110	4.5222100	1.0707360
H	2.9685130	5.7874640	1.0283130
C	4.6836380	4.5969460	-0.6893420
H	5.4084520	3.7914010	-0.9454850
H	4.4117970	5.1162850	-1.6270420
H	5.1861540	5.3088970	-0.0181400
N	-2.2461920	2.1807930	-4.2876460
H	-1.3537040	1.9105300	-3.7487960
C	-1.8539960	2.7415820	-5.6254770
H	-1.4348600	1.9477010	-6.2691010
H	-2.7053680	3.1968810	-6.1555420
H	-1.0567960	3.5183790	-5.5246290
C	-3.0202740	3.1680910	-3.4592880
H	-3.8916130	3.5730360	-3.9939000
H	-3.3894670	2.6631210	-2.5346460
H	-2.3762530	4.0135590	-3.1311160
H	-2.8307460	1.2904370	-4.4079920
S	-3.5999770	-0.6332860	-2.3535770
O	-3.4785380	-0.1747340	-3.7483280
O	-4.8582470	-1.2482420	-1.9261050
O	-3.4993990	0.8057690	-1.5063230
O	-2.3898670	-1.3818880	-1.9047200
H	-4.1049160	0.8870510	-0.6798960
S	1.8037720	2.0375770	2.7583680
O	1.6176090	1.3583380	4.0355780
O	0.8933510	3.1825110	2.5289640
O	1.3126600	0.8984000	1.6354120
O	3.2005410	2.2976520	2.3107710
H	2.0310820	0.6445940	0.9217460
H	-0.6961770	3.4207930	3.2784990
N	-1.5832380	2.9756830	3.6705590
H	-1.9009330	2.2193970	2.9517370
C	-2.6733900	4.0012150	3.8040690
H	-2.5103130	4.6874660	4.6485260
H	-2.7553440	4.6004120	2.8802000
H	-3.6714290	3.5106980	3.9433650
C	-1.2701600	2.3141630	4.9831810
H	-2.1067440	1.6803380	5.3264670
H	-0.3653250	1.6666910	4.8807530
H	-1.0485540	3.0455470	5.7779540

S	-4.3017940	1.0708140	2.1082470
O	-4.9159230	2.0843100	2.9391160
O	-4.9302390	0.7800450	0.7766510
O	-4.4743350	-0.3713790	2.9138460
O	-2.8285110	1.2758520	1.9623560
H	-4.0419360	-1.1730360	2.4620630
H	-5.9127130	-0.6177660	0.3215260
N	-6.2081130	-1.6444660	0.2479910
H	-5.3372320	-2.1503410	-0.0786850
C	-6.6292790	-2.1552180	1.5970150
H	-7.4719660	-1.5773520	2.0108870
H	-6.9112390	-3.2192390	1.5682110
H	-5.7763390	-2.0578690	2.3136340
C	-7.3057120	-1.7921670	-0.7684910
H	-6.9204880	-1.4762970	-1.7698180
H	-7.6413150	-2.8366220	-0.8662070
H	-8.1763570	-1.1636310	-0.5240890
S	-2.3796300	-2.9388020	1.0511240
O	-2.2977910	-3.9629860	0.0022330
O	-1.2739820	-1.9719380	1.0423160
O	-2.1189680	-3.8166010	2.4692950
O	-3.7216500	-2.3309930	1.2388050
H	-2.2292010	-4.7739480	2.3919360
H	2.4919380	-2.6481270	2.2928890
N	2.2361450	-1.7139730	2.7350690
H	2.2704770	-1.0002020	1.9485550
C	0.8452500	-1.7697150	3.2985440
H	0.7344750	-2.5582220	4.0575790
H	0.5600110	-0.7992420	3.7536320
H	0.1027780	-1.9770950	2.4863040
C	3.2396790	-1.3339330	3.7882590
H	4.2122600	-1.0636360	3.3233740
H	2.9015360	-0.4375200	4.3600210
H	3.4081730	-2.1482060	4.5085600
S	4.7330040	0.4421380	0.5367840
O	4.7044400	1.7763020	-0.0647560
O	3.3625330	-0.1808470	0.6056860
O	5.1359200	0.6152710	2.1423050
O	5.7298610	-0.5012690	0.0075820
H	4.7211580	1.4213740	2.5878850
N	6.4170580	-2.5890270	-1.1938490
C	6.5546870	-3.4437000	-2.4223020
H	7.0303760	-4.4138920	-2.1991180
H	5.5359020	-3.6774190	-2.8153140
H	7.1358550	-2.9446000	-3.2126400
C	7.7071080	-2.4633960	-0.4329670

H	8.5332490	-2.1097920	-1.0718870
H	7.5746380	-1.7046580	0.3765480
H	8.0081050	-3.4163880	0.0296790
H	5.6543800	-2.9896770	-0.5679940
H	6.0684270	-1.6251630	-1.4500870

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>8</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>8</sub>]<sup>+</sup>**

S	0.4452440	2.5190550	1.7473110
O	1.8416730	2.8782880	1.9903630
O	-0.4881190	3.4523900	2.7933440
O	0.0222420	1.1773260	2.2038310
O	-0.0771830	3.0434470	0.4344700
H	-1.2498850	3.9476360	2.3654380
H	2.4239590	1.2983260	-3.4540510
S	4.2939230	1.5321940	-2.1150650
O	4.2718540	2.5518840	-1.0534200
O	3.8344860	0.1753030	-1.6846920
O	5.4463580	1.4715350	-2.9800820
O	2.9435130	2.0394780	-3.0448230
O	4.9464160	-1.9984880	2.6977340
H	5.7527560	-2.5315270	2.7007660
S	4.6423490	-1.1813320	1.2273430
O	5.6687660	-1.7252080	0.3372470
O	4.7828940	0.2325970	1.5870430
O	3.2432170	-1.6043990	0.9676790
S	1.8552100	-3.0779060	-0.6207840
O	3.1627990	-3.0512740	-1.2817510
O	0.7723190	-3.5867870	-1.4869960
O	1.3431650	-1.4212920	-0.5219360
O	1.7645270	-3.5754550	0.7600900
H	1.7942100	-0.9057140	0.2330590
H	2.2703430	-0.4580420	-1.9403670
O	0.7852540	0.9309380	-0.2389940
S	0.2415780	0.5222190	-1.5191390
O	-0.8301530	-0.6877320	-1.3735220
O	1.4796290	0.0116900	-2.4620650
O	-0.3880100	1.5386010	-2.3455260
H	-0.5958730	-1.4053190	-0.6518920
S	-4.8333920	-1.4305530	-2.2261530
O	-5.1001020	-0.3732720	-3.2245720
O	-5.9659350	-1.8069160	-1.3888040
O	-3.8996410	-2.4917320	-2.6036240
O	-3.9289230	-0.4988390	-1.0910470
H	-2.9583990	-0.6386060	-1.0549960
S	-2.1396450	-2.4126480	1.7665820

O	-1.0797970	-2.5495230	2.7819550
O	-3.1948840	-1.4788120	2.1772960
O	-2.8873090	-3.9385220	1.8013200
O	-1.7223510	-2.3206750	0.3575860
H	-2.5794020	-4.5323990	2.4996960
H	-1.5865680	2.6211740	-0.1345480
S	-3.6506580	2.6844370	0.9031720
O	-4.8128380	2.9731500	0.0323850
O	-2.9925070	3.7587760	1.6548780
O	-2.5279790	2.2447600	-0.2483970
O	-3.8960530	1.5021050	1.7716860
N	-2.2217110	0.8206910	3.7865560
C	-2.0052270	-0.2695560	4.7968810
C	-2.6537000	2.1018460	4.4440650
H	-1.5762750	-1.1725320	4.2964350
H	-1.3082490	0.0399700	5.5911530
H	-2.9512080	-0.5821740	5.2690160
H	-2.8206550	2.8891330	3.6654110
H	-3.5931600	1.9868430	5.0039850
H	-1.8746060	2.4990150	5.1166670
H	-1.3087370	0.9927890	3.2379310
H	-2.9457870	0.5156740	3.0588610
N	-5.5112170	-0.4991370	1.2574400
C	-6.6054360	0.3541030	0.6777640
C	-6.0191820	-1.8758180	1.5865970
H	-6.2105060	1.3607810	0.4096400
H	-7.0049490	-0.1134290	-0.2499350
H	-7.4405200	0.4930830	1.3790780
H	-5.2060600	-2.4802440	2.0373460
H	-6.8709990	-1.8529010	2.2795860
H	-6.3437490	-2.3960360	0.6524940
H	-4.7053360	-0.5723280	0.5600890
H	-5.0880420	-0.0408090	2.0986270
N	4.5203250	2.7113830	1.6903260
C	5.2823990	2.5422400	2.9755930
C	4.3388580	4.1646320	1.3492520
H	5.4104030	1.4532650	3.1823190
H	6.2873910	2.9889980	2.9222400
H	4.7413130	2.9892190	3.8258130
H	4.0558840	4.2485350	0.2706570
H	3.5150560	4.6002630	1.9482650
H	5.2555400	4.7515260	1.5044350
H	5.0046430	2.2082220	0.9013130
H	3.5694050	2.2425290	1.7729810
N	1.2725920	3.9178050	-1.7891460
C	0.1467250	4.4583270	-2.6244090

C	2.2836950	4.9721570	-1.4464050
H	-0.5393210	3.6158950	-2.8827780
H	-0.4400250	5.2129470	-2.0741970
H	0.5045370	4.9051120	-3.5657800
H	3.1644130	4.4841040	-0.9456430
H	2.6723270	5.4836640	-2.3435210
H	1.8679580	5.7310160	-0.7639510
H	0.8608650	3.4863220	-0.8779680
H	1.7612880	3.1304330	-2.3213950
N	-4.5876160	2.2616790	-2.6840350
C	-3.2104820	2.5797820	-3.1899380
C	-5.6535930	2.9871610	-3.4560460
H	-2.4449770	2.1196730	-2.5067300
H	-3.0363010	2.1560380	-4.1931060
H	-3.0183680	3.6611240	-3.2188590
H	-6.6533500	2.7133870	-3.0680310
H	-5.5503180	4.0819620	-3.3723750
H	-5.6343050	2.7131660	-4.5266190
H	-4.7532040	1.1909780	-2.7721830
H	-4.6553890	2.5218050	-1.6420640
N	-1.8245870	-3.9246040	-1.7699550
C	-1.5141460	-4.0945950	-3.2333200
C	-2.8348920	-4.9270240	-1.2872460
H	-0.5917590	-3.5250580	-3.4736180
H	-1.3302420	-5.1454600	-3.5001000
H	-2.3488910	-3.7035950	-3.8506340
H	-3.0226570	-4.7855320	-0.2005520
H	-3.8041610	-4.7787690	-1.8079330
H	-2.5018720	-5.9621210	-1.4513660
H	-0.9256170	-3.9888530	-1.2019880
H	-2.2112710	-2.9532660	-1.6168680
N	5.3330430	-2.1697110	-2.2035230
C	6.6323330	-1.4305460	-2.3614080
C	4.9935000	-2.9867870	-3.4179250
H	6.9777680	-1.0843930	-1.3615140
H	7.4253200	-2.0570420	-2.7934430
H	6.5111190	-0.5241250	-2.9952580
H	4.0101360	-3.4873260	-3.2491790
H	4.9047010	-2.3588190	-4.3194200
H	5.7421300	-3.7703850	-3.6119640
H	5.3597280	-2.7823530	-1.3439470
H	4.5440340	-1.4798540	-2.0009800
N	1.6941640	-2.5377820	3.0871870
C	1.5930400	-1.1365370	3.6148600
C	2.4302410	-3.4426420	4.0331390
H	1.0500870	-0.4890230	2.8780290

H	1.0386890	-1.0901370	4.5621270
H	2.5904700	-0.6881300	3.7616310
H	2.4570200	-4.4693610	3.6201960
H	3.4847310	-3.1100590	4.1428750
H	1.9660530	-3.4786470	5.0294200
H	0.7273910	-2.9168170	2.8820710
H	2.2172370	-2.5403020	2.1259140

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>8</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>9</sub>]<sup>+</sup>**

S	1.0853660	-0.5015040	3.0797590
O	0.2413520	0.6910220	2.8530800
O	0.3339410	-1.7026560	3.4554730
O	2.0634840	-0.1487400	4.3827350
O	2.0898240	-0.7826400	2.0014850
H	2.1093480	0.8394640	4.6054190
N	3.6940670	2.5097390	0.6283770
H	4.0767720	2.2255900	-0.3149740
H	2.6275750	2.4996050	0.5371920
C	4.1226690	1.5284760	1.6790390
H	5.2167060	1.4918180	1.7866410
H	3.6709530	1.7719440	2.6668630
H	3.7642050	0.5046710	1.4074180
C	4.1389360	3.9119910	0.9453870
H	3.8948350	4.5726820	0.0874380
H	3.6175440	4.3069700	1.8392400
H	5.2252310	3.9730130	1.1221320
S	0.7955580	2.9566720	2.8143180
O	1.8004800	2.2825390	3.6549330
O	1.0679530	2.9313040	1.3549870
O	1.2172840	4.6029240	3.0539930
O	-0.6340570	2.9624130	3.2066740
H	1.0559060	4.9685760	3.9278110
N	-2.4528830	0.7272490	3.7166180
H	-1.5482560	1.2861250	3.6339100
H	-2.6646790	0.3681090	2.7241740
C	-2.2834710	-0.4400180	4.6455220
H	-2.1240430	-0.1294920	5.6868110
H	-3.1591990	-1.1254630	4.6031430
H	-1.4233400	-1.0742120	4.3278820
C	-3.5720430	1.6228610	4.1734850
H	-3.7970750	2.3684540	3.3829200
H	-4.5034230	1.0535470	4.3481390
H	-3.3125180	2.1635240	5.0972080
H	1.2820360	4.0216900	-0.6860120
N	0.3642720	4.5334150	-0.5129830

C	-0.3596170	4.7509920	-1.8102780
H	-0.5280210	3.7646940	-2.3225570
H	-1.3525340	5.2061740	-1.6540120
H	0.2150680	5.3810370	-2.5092050
C	0.6280900	5.8276310	0.2051270
H	-0.3100720	6.3749190	0.4107610
H	1.0964450	5.6199390	1.1977170
H	1.2974240	6.4888500	-0.3664870
H	-0.2097640	3.8960520	0.1214530
S	2.5884580	2.8341850	-3.0030230
O	2.6906170	3.2343700	-1.5739110
O	3.4257110	1.6280800	-3.3130490
O	3.4065800	4.0444510	-3.8202820
O	1.2277400	2.8312150	-3.4971310
H	4.0704290	3.7503660	-4.4653410
S	-3.0466460	2.8775450	0.2912240
O	-2.4369360	2.6579360	-1.0051700
O	-4.1878930	4.0473010	0.2800540
O	-3.2816380	1.8341420	1.2685400
O	-1.9075500	3.8347810	1.0490050
H	-1.6919730	3.5757760	2.0269350
H	-5.0765750	3.7544030	-0.1170810
H	-2.9445020	1.4022220	-2.4489560
N	-2.5469920	1.0863550	-3.3776900
C	-3.3537820	1.6984920	-4.4902710
H	-3.0161990	1.3469760	-5.4793400
H	-4.4200570	1.4043100	-4.3695300
H	-3.2989670	2.7993570	-4.4764860
C	-1.0939730	1.4559310	-3.4562380
H	-0.4613800	0.6954980	-2.9435470
H	-0.7131560	1.5345280	-4.4870730
H	-0.8948240	2.4327330	-2.9583830
H	-2.6608930	0.0266860	-3.4040330
S	-0.7207770	-2.2972380	-3.0290780
O	-2.0290010	-1.6352430	-3.3010780
O	-0.3555830	-3.3738900	-3.9233500
O	-1.0183580	-2.9660150	-1.5085380
O	0.3832470	-1.3430290	-2.7591220
H	-0.3384640	-2.7410460	-0.8202570
H	2.0951480	-1.8769240	-2.8980790
N	2.9391030	-2.2515970	-3.4389430
H	3.7593470	-2.2592790	-2.7706820
C	3.2374530	-1.3299610	-4.5889700
H	4.2151440	-1.5591500	-5.0470940
H	2.4566980	-1.3784330	-5.3650250
H	3.2879560	-0.2742800	-4.2281330



C	2.6549020	-3.6556520	-3.8954150
H	2.5906980	-4.3369460	-3.0228720
H	1.6666980	-3.7276420	-4.4121660
H	3.4306940	-4.0401690	-4.5742710
S	5.7683800	-0.4891560	-1.2985270
O	4.9210240	-1.0891600	-0.0326080
O	7.0998380	-0.2839760	-0.8375990
O	5.0217290	0.9563370	-1.4345560
O	5.4092130	-1.2541070	-2.4708930
H	4.4667000	1.1254190	-2.3483450
N	4.3281270	-2.2771820	2.9979420
H	3.5380310	-1.7636990	2.4787190
C	5.6010740	-1.4864740	2.9146860
H	6.4641570	-2.0417190	3.3201690
H	5.8283760	-1.2496660	1.8462890
H	5.5278900	-0.5309940	3.4611720
C	3.9097570	-2.5292990	4.4190520
H	3.5661200	-1.5911600	4.9124790
H	3.0515530	-3.2301720	4.4408580
H	4.7199760	-2.9626960	5.0264340
H	4.4394620	-3.1993930	2.4881490
S	-4.1312700	-2.0752820	1.7251550
O	-3.3702670	-2.6017190	2.8907950
O	-3.9706490	-2.9262500	0.5299340
O	-3.1910490	-0.7020980	1.4113730
O	-5.4735240	-1.5552440	1.9855420
H	-3.6592830	0.0315410	0.9050330
H	-1.8932800	-3.3616240	2.6496300
N	-0.9962240	-3.7920110	2.2134090
H	-0.3786850	-2.9849430	1.9273000
C	-1.3564760	-4.6153520	1.0101260
H	-0.4617970	-4.9086830	0.4176050
H	-1.9018560	-5.5314460	1.2853850
H	-2.0275020	-4.0314740	0.3256560
C	-0.2723690	-4.5989850	3.2563460
H	0.6045350	-5.1232360	2.8368090
H	0.0929920	-3.9135490	4.0522580
H	-0.9346230	-5.3491080	3.7191950
H	4.1612360	-1.8078670	-0.2986520
S	2.3501410	-3.6263710	0.1501940
O	3.1632400	-2.8120660	-0.8312360
O	1.6830170	-4.7859560	-0.3780410
O	1.0576680	-2.5740810	0.4584130
O	3.0532260	-3.7412600	1.4357680
H	1.3540810	-1.6237770	0.6551770
S	-5.5691130	0.8201980	-1.2222300

O	-4.8427370	2.0214320	-0.6605280
O	-6.9914900	0.9558790	-1.3299890
O	-5.2716770	-0.3766960	-0.0748260
O	-4.8117090	0.2869660	-2.3744670
H	-5.9903260	-0.5392650	0.6358040
N	-4.3131560	-2.6908670	-2.0858120
H	-3.5355570	-2.0739000	-2.4820240
H	-4.5404690	-2.3151500	-1.1122460
C	-5.5193680	-2.6026020	-2.9764820
H	-5.3425130	-3.0777310	-3.9561420
H	-6.4043380	-3.0751760	-2.5189390
H	-5.7594990	-1.5308690	-3.1684840
C	-3.8101230	-4.1025800	-1.9500200
H	-3.4773770	-4.5188170	-2.9137180
H	-2.9383260	-4.1030880	-1.2463490
H	-4.5727490	-4.7643360	-1.5077910

**[H((CH<sub>3</sub>)<sub>2</sub>NH)<sub>8</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>10</sub>]<sup>+</sup>**

S	3.6259210	0.5193170	-2.9412660
O	2.9554930	1.7406810	-3.3876610
O	4.9924280	0.7503990	-2.4036470
O	3.9428240	-0.3647520	-4.3608130
O	2.7833870	-0.4480430	-2.2120130
H	4.8063780	-0.2064710	-4.7642370
N	1.8454660	-2.8479570	-3.1897770
H	1.5921630	-3.4869080	-2.3814460
H	2.0437710	-1.8816360	-2.7622740
C	0.6953800	-2.7528850	-4.1489790
H	-0.2053900	-2.3081950	-3.6545280
H	0.9330410	-2.1059940	-5.0104220
H	0.3944950	-3.7394530	-4.5356420
C	3.0926150	-3.3423400	-3.8674830
H	3.4729650	-2.5953780	-4.5937440
H	3.9081220	-3.4782540	-3.1113730
H	2.9407060	-4.3011170	-4.3821480
S	-2.9182670	-0.5975670	-4.2226370
O	-2.2309130	0.6953930	-4.3564950
O	-2.0901630	-1.6715990	-3.6139580
O	-3.1049620	-1.0804970	-5.8233980
O	-4.2693160	-0.5672820	-3.6514080
H	-2.9152280	-0.3998000	-6.4853740
N	-0.7890690	2.6679460	-3.1422100
H	-1.3886100	1.7882510	-3.0853210
H	-0.2669470	2.7308330	-2.2235900
C	0.1687120	2.5555240	-4.2926600

H	-0.3039870	2.0184570	-5.1367850
H	0.5220100	3.5334850	-4.6500040
H	1.0806890	1.9815690	-3.9918520
C	-1.7004590	3.8576490	-3.2847930
H	-2.2980830	3.7942710	-4.2104910
H	-2.4100380	3.8767930	-2.4287520
H	-1.1429150	4.8070830	-3.2795180
N	-3.0012310	-3.2573110	-1.5645130
H	-2.8901090	-2.8381680	-0.5704580
H	-2.5911440	-2.5481680	-2.2646770
C	-4.4632910	-3.4485540	-1.8553980
H	-4.6353570	-3.7299840	-2.9074730
H	-4.9134310	-4.2144910	-1.2026300
H	-5.0131340	-2.4893910	-1.6643310
C	-2.2501930	-4.5519840	-1.6685190
H	-2.4260490	-5.0573860	-2.6323050
H	-1.1508720	-4.3716780	-1.5959160
H	-2.5169720	-5.2499430	-0.8574150
S	1.2113940	-4.6498360	0.2693000
O	0.7918360	-4.5267740	-1.1154050
O	2.4810680	-5.2099520	0.6859030
O	0.1414100	-5.8159770	0.8789350
H	0.5797930	-6.6131760	1.2313020
O	0.5436640	-3.5032060	1.2273970
H	0.9624640	-2.5713710	1.1573350
S	-3.2543470	1.4516300	-0.4042690
O	-4.4816140	1.7793250	-1.1423590
O	-3.2154710	0.0404740	0.0337480
O	-3.3216670	2.3099950	1.0313300
O	-2.0303010	1.9699620	-1.0586310
H	-2.9755580	3.2605000	0.9921650
H	-3.2005410	1.3969680	2.6211520
N	-2.6918780	1.1348190	3.5190400
H	-2.3513610	0.1366860	3.3701550
C	-3.6675680	1.1593350	4.6635160
H	-4.0732560	2.1707690	4.8333660
H	-4.5185380	0.4855000	4.4227990
H	-3.2025980	0.8129450	5.6011230
C	-1.5238640	2.0446410	3.7553480
H	-0.8826470	1.6933860	4.5918690
H	-0.8642950	2.0742430	2.8563360
H	-1.8337150	3.0831910	3.9737930
S	0.4566790	-0.9647690	3.9525150
O	0.8675000	0.1914040	4.7301950
O	1.0647800	-2.2596360	4.2590680
O	1.1321780	-0.6795170	2.4136270

O	-1.0205050	-1.0650150	3.7425510
H	0.9761260	0.2296200	2.0304220
H	-1.9561620	-2.5133270	3.7101100
N	-2.2012910	-3.4605790	3.2688030
H	-2.3694380	-3.2531180	2.2327970
C	-3.4542510	-4.0163860	3.8832060
H	-3.6798420	-5.0298530	3.5113980
H	-3.3901630	-4.0567110	4.9816500
H	-4.3370970	-3.3840450	3.6116050
C	-1.0419970	-4.4003270	3.4358760
H	-0.0750880	-3.8362120	3.3460350
H	-1.0262790	-4.8823650	4.4247300
H	-1.0294400	-5.1791880	2.6508770
S	3.8952410	-2.6263910	-0.0373650
O	2.3990570	-2.9514920	-0.0936090
O	4.5535450	-3.0012470	-1.2605140
O	4.4176280	-3.5888750	1.2146920
O	4.1000080	-1.2692620	0.5307040
H	4.1298300	-4.5478990	1.1695240
H	6.1483060	-0.2610140	-1.5383450
S	5.2993000	0.8967340	0.1981400
O	5.2604640	0.6238190	1.6179670
O	5.7918880	2.1972750	-0.2154790
O	3.7661810	0.9042760	-0.4290440
O	6.1441250	-0.2896250	-0.5192160
H	3.1612420	0.1279480	-0.1674310
S	1.0155420	3.4305610	0.8646670
O	2.3437090	3.7207900	0.3225140
O	0.7990740	2.1548860	1.5444430
O	0.0591740	3.4274630	-0.5049180
O	0.4725840	4.5897220	1.6702930
H	-0.9313720	3.2700280	-0.3299540
H	3.6046810	3.3457860	-0.9284750
N	4.3578230	3.8852890	-1.4614150
C	3.7567700	4.5154540	-2.6839090
H	2.9521930	5.2214820	-2.4164530
H	4.5062910	5.0510210	-3.2864550
H	3.3018690	3.7199390	-3.3272920
C	4.9582840	4.9094800	-0.5344950
H	5.6078940	4.3894930	0.2066620
H	5.5724380	5.6505040	-1.0650090
H	4.1635280	5.4277480	0.0359580
H	5.0941900	3.1754590	-1.7304240
N	4.0012310	-0.9605970	3.2497390
H	3.1467690	-0.9228000	2.6300270
C	4.0500340	-2.2739710	3.9752820

H	4.2394200	-3.1004980	3.2554800
H	4.8424010	-2.3010680	4.7376230
H	3.0764580	-2.4998820	4.4763140
C	3.9882110	0.2131290	4.1910830
H	4.7704150	0.1361080	4.9616350
H	4.1774630	1.1456820	3.6178480
H	3.0054660	0.3257850	4.7048200
H	4.8288680	-0.8762190	2.5849440
S	-1.7347740	5.6568460	1.8709400
O	-1.8512380	4.5076400	0.9628030
O	-2.9139590	6.4052010	2.1437790
O	-0.5888460	6.6895460	1.3345790
O	-1.1682130	5.1043890	3.3151690
H	0.3334990	6.2773620	1.2130610
H	-0.2199530	4.7421920	3.2881940
S	-4.4710820	-1.4517910	1.2678800
O	-5.3975910	-1.1979870	0.1459640
O	-3.3640440	-2.4252710	0.9901920
O	-5.4583470	-2.5442050	2.1816190
O	-4.2130390	-0.4397920	2.2869760
H	-6.4025600	-2.4581130	2.0548470
N	-6.2770110	0.3172620	-1.9599300
H	-5.3780520	0.4106340	-2.5273310
C	-7.0171300	-0.9225800	-2.3751340
H	-6.4657950	-1.8080050	-1.9811360
H	-8.0393720	-0.9561180	-1.9685290
H	-7.0605680	-1.0134390	-3.4747170
C	-7.1038160	1.5607860	-2.1244660
H	-8.0062730	1.5445540	-1.4936740
H	-6.4885930	2.4394950	-1.8132990
H	-7.4081120	1.7163650	-3.1716070
H	-5.9541430	0.2239570	-0.9476520



S	1.9250140	-1.0405720	4.7050690
O	0.5250740	-0.9616730	4.2415260
O	2.4496330	-2.4116990	4.7582860
O	1.7093100	-0.6262350	6.3419890
O	2.8254150	-0.0157880	4.1774560
H	2.3807220	-0.9464350	6.9537600
N	3.7569100	1.3317630	2.0954690
H	3.5795990	1.4286550	1.0590940
H	3.2373380	0.4662380	2.4376940
C	3.2138070	2.5472370	2.8004570
H	2.1743490	2.7491200	2.4672850

H	3.2000790	2.3861800	3.8941040
H	3.8130000	3.4476330	2.5618310
C	5.2329180	1.1701790	2.3374350
H	5.4458730	1.0183650	3.4099920
H	5.6294520	0.2966720	1.7845370
H	5.7918890	2.0597250	1.9810160
S	-0.9639740	3.8128770	2.6882480
O	-1.1469930	2.7082990	3.6311220
O	0.1411050	3.6456780	1.6929510
O	-0.3842410	5.0524520	3.6690340
O	-2.1695990	4.3677920	2.0695660
H	-0.2384580	4.8211500	4.5970570
N	-1.6507550	0.2082060	4.5778000
H	-1.0507700	0.8254390	3.9602140
H	-1.3779990	-0.7809840	4.3465030
C	-1.3326770	0.5069290	6.0189040
H	-1.4274890	1.5871220	6.2263670
H	-1.9863000	-0.0441460	6.7119240
H	-0.2799340	0.2123790	6.2471660
C	-3.1012810	0.4420310	4.2764640
H	-3.3228670	1.5225630	4.2155790
H	-3.3801590	-0.0014160	3.2812610
H	-3.7703200	-0.0176680	5.0185840
N	-0.0257560	5.2507930	-0.5851520
H	-0.3912370	4.5248860	-1.3054380
H	0.2998760	4.6986880	0.2699850
C	-1.1571020	6.1587980	-0.1914380
H	-0.8431280	6.9214640	0.5405130
H	-1.5939750	6.6693710	-1.0659750
H	-1.9692010	5.5581450	0.2886480
C	1.1237390	6.0177080	-1.1697080
H	1.5597190	6.7305760	-0.4487380
H	1.9439040	5.3192130	-1.4636710
H	0.8276390	6.5784930	-2.0714080
S	4.3128970	3.5705800	-1.0169830
O	4.6018000	3.5333800	0.3831790
O	5.1993050	3.1112530	-2.0731040
O	4.1369920	5.2001400	-1.4241360
H	4.7647200	5.5287290	-2.0929400
O	2.7293690	3.2938340	-1.3368920
H	2.3177020	2.4665350	-0.8459720
S	-4.7210910	0.1812410	0.5806310
O	-5.0104340	1.5385700	1.0646440
O	-3.9358450	0.1018830	-0.6482370
O	-6.2084540	-0.4634130	0.2601720
O	-4.1273310	-0.6805620	1.6738340

H	-6.2163000	-1.4073900	-0.0665610
S	5.0542880	0.3401580	-1.3911620
O	4.1109130	1.3875150	-0.8285280
O	6.3296410	0.3029440	-0.7444940
O	5.1757380	0.7453930	-2.9974010
O	4.3478010	-0.9924480	-1.4938030
H	5.5417760	1.6659040	-3.1640420
N	-3.4535860	-0.4139020	-3.2361600
H	-2.4212130	-0.2280510	-3.3934580
C	-4.2009190	-0.1450170	-4.5141970
H	-5.2809650	-0.3336080	-4.4000620
H	-4.0667210	0.9203040	-4.7961410
H	-3.8278440	-0.7768610	-5.3385970
C	-3.6571440	-1.8236620	-2.7613970
H	-3.2566080	-2.5686620	-3.4799740
H	-3.1392220	-1.9795860	-1.7859940
H	-4.7212200	-2.0512240	-2.5672820
H	-3.7671210	0.2761390	-2.4898490
H	0.2258380	-1.8985790	-1.9442950
S	-0.2946630	-2.1090400	-4.2131060
O	-1.3674470	-3.0241630	-4.5149500
O	0.9492920	-2.1899080	-5.0010910
O	0.3287790	-2.5586100	-2.7002420
O	-0.7383780	-0.6897140	-4.0112200
H	0.3215550	0.6229610	-4.1525060
N	1.2534530	1.0586490	-3.8201540
H	1.3571200	0.7500600	-2.8126400
C	1.1774220	2.5539950	-3.8816570
H	2.0400120	3.0321700	-3.3795280
H	1.1190520	2.9275060	-4.9142070
H	0.2574320	2.9113930	-3.3444860
C	2.3918470	0.5168540	-4.6361460
H	2.2864150	-0.5939680	-4.7529280
H	2.4106630	0.9374170	-5.6540020
H	3.3758690	0.7162810	-4.1628650
H	6.0687450	-4.2685500	0.8944930
S	3.8563380	-3.9780870	0.4925970
O	3.3624510	-4.2793610	-0.8316640
O	3.0359520	-4.2796280	1.6331250
O	4.4958170	-2.5256880	0.5267290
O	5.2795440	-4.8125820	0.6915250
H	4.2857530	-1.8365590	-0.3314090
H	-2.8648040	-1.4225690	1.5911990
S	-1.1338020	-2.7570690	0.6664450
O	-0.5274260	-3.8027680	1.4707840
O	-0.1543720	-1.8206080	0.0068570

O	-1.8019970	-1.6528640	1.7366370
O	-2.2480910	-3.1542300	-0.2101670
H	2.0192930	-3.8321580	3.7648430
H	1.0701330	-4.2709990	2.4110420
N	1.2305720	-4.4788020	3.4409110
C	-0.0272840	-4.1760410	4.2082810
H	-0.8966040	-4.6961490	3.7646190
H	0.0638940	-4.4443460	5.2710990
H	-0.2408860	-3.0841080	4.1436040
C	1.6530870	-5.9124140	3.6021430
H	2.5650670	-6.0947240	2.9944830
H	1.8918150	-6.1521670	4.6515800
H	0.8719330	-6.6095730	3.2536430
H	3.2809410	-4.4488540	-2.6527860
N	2.7548430	-3.8827970	-3.3640810
H	1.9351540	-3.4225360	-2.8536520
C	3.6443400	-2.8064620	-3.9190540
H	4.0241830	-2.1564780	-3.0928990
H	4.5084730	-3.2129380	-4.4632330
H	3.0679770	-2.1503550	-4.6166730
C	2.2316210	-4.7818850	-4.4501530
H	3.0360810	-5.3440260	-4.9483560
H	1.4965770	-5.4997170	-4.0444580
H	1.7027690	-4.1801810	-5.2328080
S	-5.6041290	-4.4601430	-0.4255580
O	-5.6250880	-3.0379380	-0.6696960
O	-6.6302510	-5.1442740	0.2841330
O	-4.1725930	-4.8918350	0.1800560
O	-5.5005300	-5.1535910	-1.9339970
H	-3.3381320	-4.3064920	-0.0724380
H	-5.8356080	-6.0648520	-2.0183980
S	-2.7169330	3.4146420	-2.4640270
O	-3.4133190	3.8339050	-1.2435290
O	-1.2359730	3.5266700	-2.3254250
O	-3.0762560	4.6619030	-3.5543040
O	-3.1877180	2.2259000	-3.1703800
H	-3.4894190	4.3864080	-4.3816400
H	-5.0551460	3.2641070	0.3724040
N	-4.7091590	4.1050260	0.9189130
H	-3.6519950	4.0469600	0.8693160
C	-5.1795150	5.3789510	0.2747380
H	-4.7822200	5.4282710	-0.7658020
H	-6.2789350	5.4275020	0.2180670
H	-4.8197350	6.2671880	0.8183540
C	-5.1542820	4.0086040	2.3532410
H	-6.2016300	4.3175770	2.4876810



H	-5.0830630	2.9449800	2.6795980
H	-4.5033340	4.6155030	3.0065690
S	0.9188080	0.0808630	0.1845160
O	1.9015340	-0.5938650	0.9884040
O	1.4401060	1.7027510	0.3485050
O	-0.4525740	0.4593640	0.9564800
O	0.8487360	-0.0430980	-1.2561360
H	-1.0591160	-0.2999860	1.3638240
H	0.7929700	2.3316660	0.8307970