Supporting Information

Characterization of the Nucleation Precursor (H_2SO_4-$(CH_3)_2NH$) Complex: Intra-cluster Interactions and Atmospheric Relevance

Yan Ma,[1] Jiao Chen,[1] Shuai Jiang,[1] Yi-Rong Liu,[1] Teng Huang,[1] Shou-Kui Miao,[1] Chun-Yu Wang,[1] Wei Huang*[1,2]

[1]*Laboratory of Atmospheric Physico-Chemistry, Anhui Institute of Optics & Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui 23 0031, China*

[2]*School of Environmental Science & Optoelectronic Technology, University of Science and Technology of China, Hefei, Anhui 230026, China*

*E-mail: huangwei6@ustc.edu.cn

Boltzmann Averaging of Enthalpies and Free Energies

The presence of many stable structures within available thermal energy (k_bT) suggests that a meaningful free energy for a cluster of size n_i waters must include a weighted account of all isomers of $(H_2SO_4)_m[(CH_3)_2NH]_n$[m=1-2, n=1-3]. We weigh the contribution of each low energy isomer by its Boltzmann factors (x_{ni} and y_{ni}) to get the Boltzmann averaged ΔH^n_T and ΔG^n_T

$$x_{ni} = \frac{e^{-\Delta\Delta G_T^{n_i}/k_bT}}{\sum_{n_i} e^{-\Delta\Delta G_T^{n_i}/k_bT}} \quad y_{ni} = \frac{e^{-\Delta\Delta H_T^{n_i}/k_bT}}{\sum_{n_i} e^{-\Delta\Delta H_T^{n_i}/k_bT}}$$

$$\Delta G_T^n = \sum_{n_i} x_{n_i} \Delta G_T^{n_i}$$
$$\Delta H_T^n = \sum_{n_i} y_{n_i} \Delta H_T^{n_i}$$

Where

$$\Delta H_T^{n_i} = H_T^{n_i} - m_i H_T^{SA} - n_i H_T^{DMA}$$
$$\Delta\Delta H_T^{n_i} = \Delta H_T^{n_i} - \min_i \{\Delta H_T^{n_i}\}$$
$$\Delta G_T^{n_i} = G_T^{n_i} - m_i G_T^{SA} - n_i G_T^{DMA}$$
$$\Delta\Delta G_T^{n_i} = \Delta G_T^{n_i} - \min_i \{\Delta G_T^{n_i}\}$$

Table S1. The relative population fractions (RPFs) of the clusters at the temperature of 298.15 K[a], 273.15 K[b], 216.65 K[c], respectively. The estimated atmospheric relative population fractions are based on sulfuric acid concentration of $5*10^7$molecule.cm^{-3} and the dimethylamine concentration of 1ppt.

298.15 K

Clusters	RPF
$(H_2SO_4)_1[(CH_3)_2NH]_1$	$1.34*10^{-3}$
$(H_2SO_4)_1[(CH_3)_2NH]_2$	$1.74*10^{-13}$
$(H_2SO_4)_1[(CH_3)_2NH]_3$	$1.53*10^{-24}$
$(H_2SO_4)_2[(CH_3)_2NH]_1$	$1.40*10^{-3}$
$(H_2SO_4)_2[(CH_3)_2NH]_2$	$2.21*10^{-2}$

273.15 K

Clusters	RPF
$(H_2SO_4)_1[(CH_3)_2NH]_2$	$5.89*10^{-50}$
$(H_2SO_4)_1[(CH_3)_2NH]_3$	$7.81*10^{-81}$
$(H_2SO_4)_1[(CH_3)_2NH]_1$	$9.41*10^{-21}$
$(H_2SO_4)_2[(CH_3)_2NH]_1$	$4.82*10^{-42}$
$(H_2SO_4)_2[(CH_3)_2NH]_2$	$2.31*10^{-61}$

216.65 K

Clusters	RPF
$(H_2SO_4)_1[(CH_3)_2NH]_1$	$8.47*10^{-23}$
$(H_2SO_4)_1[(CH_3)_2NH]_2$	$1.07*10^{-53}$
$(H_2SO_4)_1[(CH_3)_2NH]_3$	$2.89*10^{-93}$
$(H_2SO_4)_2[(CH_3)_2NH]_1$	$1.56*10^{-46}$
$(H_2SO_4)_2[(CH_3)_2NH]_2$	$8.99*10^{-59}$

[a] The temperature of atmospheric layer, [b] The average temperature of troposphere, [c] The temperature of troposphere boundary layer.

Data S1: The coordinates of $(H_2SO_4)_m[(CH_3)_2NH]_n$ (m=1~2, n=1~3) isomers

$(H_2SO_4)[(CH_3)_2NH]_1$

Isomer I -C1

S 1.275933 -0.138164 -0.009721
O 2.391312 -1.060210 0.008442
O 0.422443 -0.176760 1.212903
O 1.921698 1.371521 -0.032646
O 0.441379 -0.132038 -1.234923
H 2.785033 1.300120 0.411359
H -1.173366 -0.036303 -0.803161

C	-2.586814	1.296269	0.021284
N	-1.879724	-0.000232	-0.006835
C	-2.747810	-1.195160	-0.002078
H	-1.843259	2.097961	0.015804
H	-3.194597	1.366236	0.928958
H	-3.231243	1.387661	-0.858931
H	-1.134010	-0.055168	0.764585
H	-2.113878	-2.085685	-0.024235
H	-3.398905	-1.185667	-0.882090
H	-3.359541	-1.203667	0.905641

Isomer I -A1

S	1.276007	-0.138557	0.009429
O	0.423871	-0.178373	-1.213856
O	2.394191	-1.057160	-0.008216
O	1.917097	1.373225	0.034901
O	0.440285	-0.136106	1.234032
H	2.780352	1.305529	-0.409827
H	-1.170544	-0.037671	0.800241
C	-2.748743	-1.194455	0.002707
N	-1.879267	-0.000554	0.005444
C	-2.584748	1.296842	-0.020779
H	-2.115772	-2.085726	0.022306
H	-3.363576	-1.201739	-0.902934
H	-3.396850	-1.184723	0.884915
H	-1.135761	-0.056161	-0.767391
H	-1.840160	2.097586	-0.015835
H	-3.227655	1.388383	0.860527
H	-3.193894	1.368289	-0.927433

Isomer I -A2

S	-1.213315	-0.147841	0.046000
O	-2.373697	-1.007911	-0.047024
O	-0.391575	-0.191111	1.251362
O	-0.342207	-0.223237	-1.189186
O	-1.780049	1.395673	0.036684
H	0.986912	-0.081635	-0.845468
H	-2.625235	1.368528	-0.445471
C	2.252355	1.294615	0.212777
N	2.095611	0.021498	-0.535332
C	2.473914	-1.179308	0.251978
H	1.956045	2.124392	-0.435082
H	3.290952	1.422504	0.537168
H	1.579628	1.255031	1.073963

H 2.646581 0.057472 -1.396630
H 2.347997 -2.066624 -0.374756
H 1.790562 -1.241025 1.103260
H 3.512936 -1.102837 0.591118

$(H_2SO_4)[(CH_3)_2NH]_2$

Isomer II -A1

S -0.05346 -0.75313 -0.01507
O 0.73208 0.01994 1.14788
O 0.88284 -1.65436 -0.65637
O -0.56009 0.31231 -0.93345
O -1.18120 -1.38997 0.69573
H 1.66961 0.20981 0.80386
H -2.58358 -0.45900 0.47578
C -4.13767 0.05424 -0.85565
H -4.97075 -0.29846 -0.24636
H -3.82859 -0.73235 -1.54257
H -4.44564 0.93346 -1.42262
N -2.98942 0.39533 0.00965
C -3.22689 1.45819 1.01174
H -2.11461 0.61466 -0.56050
H -4.03076 1.15945 1.68546
H -2.30729 1.60118 1.57749
H -3.49586 2.38639 0.50651
N 3.12663 0.29244 -0.05477
C 4.38939 0.17694 0.67421
C 3.09468 1.40216 -1.01168
H 2.92036 -0.57731 -0.54277
H 4.53487 1.06377 1.29730
H 4.35211 -0.69535 1.32939
H 5.26204 0.08103 0.01083
H 3.18358 2.34913 -0.47179
H 3.90691 1.35298 -1.75183
H 2.13646 1.39369 -1.53317

Isomer II -A2

S 1.790637 -0.230566 -0.022126
O 0.885724 -0.471920 1.111173
O 2.132080 -1.381711 -0.844029
O 1.356181 0.957178 -0.816723
O 3.180516 0.237016 0.711725
H -0.117644 1.331775 -0.434856
H 3.900121 -0.036199 0.116143
C -2.872514 -1.670251 1.013952

N	-1.778104	-1.210322	0.158349
C	-1.700224	-1.943417	-1.110750
H	-2.834887	-1.149750	1.977948
H	-2.834544	-2.756554	1.205887
H	-3.837352	-1.447285	0.539247
H	-0.878226	-1.310970	0.647306
H	-0.794407	-1.645209	-1.650448
H	-2.578254	-1.713527	-1.729135
H	-1.663970	-3.036019	-0.963199
C	-1.174161	2.143313	1.175043
N	-1.148179	1.477116	-0.145272
C	-1.877747	2.197795	-1.206438
H	-0.570719	1.545470	1.864006
H	-2.205446	2.218586	1.537568
H	-0.743065	3.146393	1.090770
H	-1.525124	0.457361	-0.042358
H	-1.786111	1.640178	-2.143107
H	-1.448536	3.196131	-1.341932
H	-2.936181	2.291971	-0.939368

Isomer II -A3

S	-0.057987	-0.297636	0.000187
O	0.811280	-1.474723	-0.000867
O	-0.910626	-0.187687	-1.223725
O	-0.911087	-0.190098	1.223943
O	0.863300	0.984653	0.001673
H	-2.431463	0.054260	0.781106
H	1.893507	0.672701	0.000914
C	4.028124	0.263313	-1.226864
N	3.263017	0.033994	-0.000249
C	4.029035	0.260981	1.226237
H	3.399103	0.034609	-2.093587
H	4.941756	-0.352194	-1.277227
H	4.322174	1.318832	-1.282447
H	2.862545	-0.910676	-0.001002
H	3.400673	0.030578	2.092987
H	4.323081	1.316403	1.283646
H	4.942728	-0.354584	1.274719
C	-4.130648	-0.948248	-0.001522
N	-3.166899	0.166907	-0.000017
C	-3.758708	1.516775	0.001136
H	-3.573127	-1.888986	-0.002025
H	-4.761213	-0.897291	-0.895676
H	-4.762258	-0.898850	0.891983

H	-2.430834	0.055827	-0.780893
H	-2.948632	2.251443	0.002152
H	-4.376727	1.653961	0.894943
H	-4.376099	1.655756	-0.892828

Isomer II -B1

S	-1.910930	-0.053795	0.149843
O	-0.905912	-0.484057	1.164789
O	-3.323541	-0.008899	0.549796
O	-1.442074	1.177424	-0.603208
O	-1.779907	-1.310452	-0.992334
H	0.123403	1.387193	-0.412395
H	-2.591950	-1.270626	-1.530783
C	1.894474	2.148868	-1.270138
N	1.174604	1.454053	-0.181336
C	1.307684	2.094111	1.149924
H	1.720683	1.613713	-2.210976
H	2.971114	2.170885	-1.055947
H	1.522575	3.176614	-1.368982
H	1.498760	0.404642	-0.100761
H	0.721287	1.505221	1.864847
H	0.913525	3.117339	1.111533
H	2.363343	2.117194	1.451012
C	1.645644	-2.028049	-1.092478
N	1.705222	-1.235042	0.145104
C	2.792734	-1.650733	1.038169
H	0.732112	-1.768305	-1.642766
H	1.627541	-3.115192	-0.892366
H	2.524326	-1.811701	-1.719170
H	0.798842	-1.316971	0.632746
H	2.737778	-1.086308	1.978985
H	3.765622	-1.444019	0.566868
H	2.755382	-2.729344	1.279084

Isomer II -B2

S	-1.914342	-0.055067	0.006024
O	-3.370373	-0.244696	-0.007089
O	-1.178806	-0.190476	1.288150
O	-1.267806	-1.405832	-0.862583
O	-1.433967	1.136387	-0.799174
H	-1.867148	-1.569604	-1.613418
H	0.095643	1.435952	-0.378569
C	2.645395	-1.774805	-0.962849
N	1.621325	-1.256957	-0.046642

C	1.752946	-1.794936	1.317915
H	2.456507	-1.405925	-1.980454
H	2.669787	-2.880004	-0.993509
H	3.640315	-1.425413	-0.648147
H	0.688723	-1.513502	-0.402010
H	0.889338	-1.465929	1.908814
H	2.677564	-1.417372	1.780656
H	1.791545	-2.899614	1.330514
C	1.936985	2.197515	-1.053829
N	1.120668	1.472730	-0.055296
C	1.172220	2.047518	1.311551
H	1.818884	1.714292	-2.030776
H	2.994977	2.177603	-0.761263
H	1.600051	3.239298	-1.127128
H	1.408473	0.410464	-0.025980
H	0.490681	1.466657	1.943031
H	0.844638	3.094632	1.284555
H	2.197877	1.994301	1.699709

Isomer II -B3

S	0.000108	0.678178	0.000027
O	-1.054177	1.418247	-0.717341
O	1.054058	1.417951	0.718215
O	-0.691944	-0.307339	1.052166
O	0.692507	-0.306010	-1.052945
H	-1.723816	-0.542186	0.736181
H	1.724434	-0.541553	-0.736636
C	-3.905322	0.391191	0.613511
N	-3.095847	-0.812306	0.333274
C	-3.105518	-1.186825	-1.095992
H	-3.887554	0.597455	1.691109
H	-4.950722	0.273722	0.281754
H	-3.446393	1.239241	0.089989
H	-3.446501	-1.595389	0.891135
H	-2.504984	-2.094026	-1.238688
H	-2.641624	-0.371901	-1.665513
H	-4.128056	-1.361838	-1.470883
C	3.905429	0.391396	-0.612826
N	3.095692	-0.812179	-0.333571
C	3.104911	-1.187609	1.095476
H	3.887854	0.598421	-1.690279
H	4.950741	0.273478	-0.280984
H	3.446539	1.239136	-0.088770
H	3.446382	-1.594967	-0.891831

H	2.504083	-2.094725	1.237440
H	2.641104	-0.372905	1.665379
H	4.127321	-1.363122	1.470458

Isomer II -C1

S	-1.790526	-0.231030	-0.021976
O	-2.131106	-1.382297	-0.844079
O	-0.885632	-0.471913	1.111408
O	-1.356648	0.957164	-0.816375
O	-3.180972	0.235653	0.711308
H	0.116457	1.331518	-0.434660
H	-3.900249	-0.040796	0.116833
C	1.875974	2.198571	-1.206725
N	1.147208	1.477475	-0.145298
C	1.173160	2.143813	1.174965
H	1.784453	1.640832	-2.143332
H	2.934421	2.293565	-0.939994
H	1.445970	3.196570	-1.342166
H	1.524762	0.458222	-0.042494
H	0.570438	1.545562	1.864194
H	0.741172	3.146505	1.090697
H	2.204516	2.220008	1.537084
C	1.701242	-1.943505	-1.110539
N	1.778937	-1.210220	0.158396
C	2.874103	-1.668886	1.013665
H	0.794977	-1.646165	-1.649963
H	1.666059	-3.036150	-0.962930
H	2.578823	-1.712898	-1.729305
H	0.879373	-1.311434	0.647698
H	2.836074	-1.148518	1.977715
H	3.838549	-1.444677	0.538742
H	2.837584	-2.755264	1.205521

Isomer II -C2

S	-1.896667	-0.105497	-0.137099
O	-3.274966	-0.052468	-0.580658
O	-0.879536	-0.508098	-1.117985
O	-1.462906	1.101410	0.628246
O	-1.819818	-1.341022	0.965358
H	0.057637	1.351603	0.389960
H	-2.702207	-1.386119	1.372996
C	2.808151	-1.609819	-1.077072
N	1.772403	-1.203726	-0.126009
C	1.814531	-1.970834	1.122325

H	2.677519	-1.069124	-2.021476
H	2.785947	-2.692047	-1.293468
H	3.801267	-1.368528	-0.674974
H	0.842227	-1.310810	-0.554578
H	0.952073	-1.704361	1.742906
H	2.736173	-1.739298	1.673184
H	1.787763	-3.060417	0.948990
C	1.217428	2.141084	-1.155206
N	1.109418	1.481205	0.164566
C	1.777991	2.206816	1.261920
H	0.663795	1.537636	-1.880065
H	2.269475	2.220567	-1.450957
H	0.775121	3.141382	-1.104229
H	1.491121	0.463486	0.086186
H	1.630744	1.655794	2.195411
H	1.343975	3.206839	1.365686
H	2.850502	2.296938	1.056621

Isomer II -C3

S	-0.058003	-0.297887	0.000151
O	-0.910811	-0.188226	1.223951
O	0.811360	-1.474901	0.001060
O	-0.910970	-0.190184	-1.223708
O	0.863192	0.984493	-0.000976
H	-2.431174	0.054558	-0.781004
H	1.893377	0.672645	-0.000487
C	-3.758445	1.517042	-0.000959
N	-3.166863	0.167073	-0.000046
C	-4.130784	-0.947927	0.000727
H	-2.948239	2.251568	-0.001372
H	-4.376186	1.655804	0.892795
H	-4.376059	1.654653	-0.894978
H	-2.431064	0.055636	0.780995
H	-3.573411	-1.888752	0.001688
H	-4.761661	-0.898453	-0.893291
H	-4.762067	-0.896858	0.894367
C	4.028369	0.261378	-1.226728
N	3.263042	0.034074	0.000114
C	4.028720	0.263386	1.226370
H	3.399626	0.030916	-2.093187
H	4.942199	-0.353947	-1.275770
H	4.322128	1.316878	-1.284178
H	2.862709	-0.910647	0.000941
H	3.400275	0.034183	2.093376

H	4.322372	1.319009	1.282087
H	4.942637	-0.351755	1.276056

Isomer II -C4

S	-1.790526	-0.231030	-0.021976
O	-2.131106	-1.382297	-0.844079
O	-0.885632	-0.471913	1.111408
O	-1.356648	0.957164	-0.816375
O	-3.180972	0.235653	0.711308
H	0.116457	1.331518	-0.434660
H	-3.900249	-0.040796	0.116833
C	1.875974	2.198571	-1.206725
N	1.147208	1.477475	-0.145298
C	1.173160	2.143813	1.174965
H	1.784453	1.640832	-2.143332
H	2.934421	2.293565	-0.939994
H	1.445970	3.196570	-1.342166
H	1.524762	0.458222	-0.042494
H	0.570438	1.545562	1.864194
H	0.741172	3.146505	1.090697
H	2.204516	2.220008	1.537084
C	1.701242	-1.943505	-1.110539
N	1.778937	-1.210220	0.158396
C	2.874103	-1.668886	1.013665
H	0.794977	-1.646165	-1.649963
H	1.666059	-3.036150	-0.962930
H	2.578823	-1.712898	-1.729305
H	0.879373	-1.311434	0.647698
H	2.836074	-1.148518	1.977715
H	3.838549	-1.444677	0.538742
H	2.837584	-2.755264	1.205521

Isomer II -C5

S	0.000055	-0.009367	0.004944
O	0.871486	-0.854263	-0.884855
O	-0.868387	-0.895339	0.854395
O	0.872887	0.843605	0.887159
O	-0.876029	0.877418	-0.842642
H	2.366748	0.541547	0.556893
H	-2.353164	0.556575	-0.528604
C	3.916101	0.907793	-0.862067
N	3.130294	0.005984	-0.005453
C	3.914965	-0.890980	0.857200
H	3.224883	1.521399	-1.446777

H 4.550457 0.326859 -1.541412
H 4.547467 1.558479 -0.246173
H 2.376656 -0.536341 -0.569407
H 3.222618 -1.508071 1.436807
H 4.540188 -0.305438 1.540928
H 4.555192 -1.537953 0.246505
C -3.921337 0.871071 0.889258
N -3.130376 0.001971 0.004022
C -3.909729 -0.853518 -0.904264
H -3.233772 1.457701 1.505155
H -4.564915 0.266024 1.538331
H -4.543842 1.548890 0.294046
H -2.390179 -0.566752 0.552326
H -3.213844 -1.441852 -1.508990
H -4.530817 -0.235424 -1.562589
H -4.553628 -1.529022 -0.329346

$(H_2SO_4)[(CH_3)_2NH]_3$

Isomers III -A1

S 0.578399 -0.890681 -0.742196
O 1.816971 -1.465311 -1.263382
O -0.505565 -0.662111 -1.701235
O 0.081971 -1.624237 0.470988
O 0.946848 0.597525 -0.210968
H -1.409766 -1.271646 0.610973
H 1.956796 0.585068 0.086869
C -3.259170 -1.620444 -0.334486
N -2.438010 -0.908394 0.667913
C -2.935111 -1.024764 2.051499
H -2.765754 -1.514041 -1.304310
H -4.268917 -1.195079 -0.365430
H -3.319839 -2.682102 -0.071842
H -2.337037 0.137290 0.392395
H -2.258817 -0.483710 2.720063
H -2.961863 -2.078493 2.349051
H -3.942958 -0.601435 2.131146
C 4.445671 1.288801 -0.127774
N 3.491190 0.290243 0.350806
C 3.765331 -0.182493 1.708480
H 4.206670 1.554864 -1.163095
H 5.490598 0.935535 -0.086130
H 4.369650 2.194934 0.487050
H 3.452727 -0.508791 -0.292376
H 3.040384 -0.959969 1.972437

H	3.655066	0.649777	2.415655
H	4.783790	-0.592881	1.819240
C	-2.426866	2.092121	-1.387774
N	-1.887640	1.740338	-0.070129
C	-2.067127	2.803676	0.918927
H	-2.153207	1.307673	-2.100471
H	-2.037719	3.056249	-1.759492
H	-3.521446	2.169902	-1.335153
H	-0.885433	1.536425	-0.173329
H	-1.578381	2.523028	1.859381
H	-3.136934	2.953646	1.117670
H	-1.648932	3.771040	0.588259

Isomers III -A2

S	2.195904	-0.523164	-0.086661
O	2.256138	0.926269	-0.425066
O	3.494451	-1.153850	0.047876
O	1.197081	-0.786975	0.957126
O	1.495581	-1.231852	-1.421229
H	-0.766701	1.613483	0.063154
H	2.239172	-1.517105	-1.980271
C	0.090318	3.551974	-0.030140
N	0.086717	2.169807	0.490251
C	0.046099	2.086602	1.966417
H	0.144385	3.522142	-1.122342
H	0.961539	4.093073	0.354151
H	-0.823676	4.072573	0.276733
H	0.966712	1.661762	0.137477
H	0.128608	1.033713	2.248773
H	-0.890920	2.515893	2.338784
H	0.892650	2.637069	2.390615
C	-3.340258	1.229081	-0.411399
N	-1.981338	0.741402	-0.652542
C	-1.671362	0.635367	-2.083341
H	-3.551535	1.225186	0.664680
H	-4.108017	0.615030	-0.914606
H	-3.447193	2.259219	-0.779121
H	-1.882401	-0.211706	-0.228716
H	-0.671440	0.204629	-2.209106
H	-1.686329	1.630870	-2.548954
H	-2.396489	0.002920	-2.624354
C	-2.098791	-2.261971	1.797174
N	-1.498910	-1.957233	0.501394
C	-1.639662	-3.057661	-0.449494

H	-1.893181	-1.448144	2.503055
H	-1.721593	-3.202593	2.241223
H	-3.188977	-2.357133	1.693812
H	-0.502035	-1.746757	0.633346
H	-1.081673	-2.825490	-1.363216
H	-2.698199	-3.193555	-0.712809
H	-1.266532	-4.021382	-0.054411

Isomers III -A3

S	-0.062274	1.898923	-0.105370
O	-0.373084	3.086290	-0.878423
O	0.525480	0.772076	-0.881481
O	1.208845	2.304876	0.869299
O	-1.119830	1.427830	0.805503
H	1.106505	3.254333	1.056426
H	0.050196	-0.665000	-0.251733
C	3.858921	-0.421696	0.982026
N	3.022497	-0.872315	-0.125636
C	3.811351	-1.349913	-1.255069
H	3.232913	0.036928	1.756098
H	4.624268	0.320754	0.681730
H	4.385483	-1.278768	1.425652
H	2.425326	-0.099389	-0.430755
H	3.151371	-1.587104	-2.098512
H	4.346801	-2.268350	-0.974785
H	4.567105	-0.620782	-1.608742
C	0.011715	-2.721765	-0.643926
N	-0.381588	-1.547527	0.163350
C	0.025008	-1.642886	1.585230
H	-0.307197	-2.567260	-1.679081
H	-0.466200	-3.623145	-0.245095
H	1.101169	-2.824013	-0.605010
H	-1.447916	-1.358443	0.099173
H	-0.278019	-0.719484	2.086984
H	1.113436	-1.752153	1.629112
H	-0.462919	-2.506589	2.050106
C	-3.473146	-0.521375	-1.402660
N	-3.012447	-0.651660	-0.017373
C	-4.071582	-1.089813	0.892250
H	-2.667540	-0.107601	-2.019858
H	-4.352217	0.139053	-1.497123
H	-3.747558	-1.507928	-1.799604
H	-2.635002	0.254561	0.292835
H	-3.697657	-1.093304	1.922501

H -4.385442 -2.110514 0.636033
H -4.964646 -0.441951 0.850885

Isomers III -C1

S 0.578402 -0.890657 -0.742220
O -0.505577 -0.662087 -1.701241
O 1.816968 -1.465286 -1.263417
O 0.946854 0.597545 -0.210985
O 0.081992 -1.624217 0.470970
H 1.956801 0.585074 0.086855
H -1.409738 -1.271650 0.610967
C -2.426918 2.092119 -1.387754
N -1.887664 1.740333 -0.070122
C -2.067136 2.803668 0.918940
H -2.153259 1.307682 -2.100461
H -2.037792 3.056257 -1.759469
H -3.521497 2.169883 -1.335114
H -0.885458 1.536424 -0.173346
H -1.578357 2.523025 1.859378
H -3.136937 2.953625 1.117716
H -1.648963 3.771036 0.588258
C -3.259153 -1.620491 -0.334461
N -2.437989 -0.908415 0.667916
C -2.935069 -1.024779 2.051510
H -2.765760 -1.514079 -1.304296
H -4.268912 -1.195156 -0.365385
H -3.319785 -2.682150 -0.071812
H -2.337037 0.137263 0.392388
H -2.258782 -0.483694 2.720056
H -2.961786 -2.078502 2.349079
H -3.942927 -0.601478 2.131163
C 4.445679 1.288817 -0.127725
N 3.491191 0.290245 0.350803
C 3.765307 -0.182536 1.708466
H 4.206704 1.554907 -1.163045
H 5.490606 0.935554 -0.086064
H 4.369640 2.194933 0.487121
H 3.452740 -0.508766 -0.292409
H 3.040363 -0.960030 1.972379
H 3.655018 0.649706 2.415669
H 4.783767 -0.592917 1.819234

Isomers III -C2

S -0.639457 -0.506169 -0.676987

O	0.450302	0.086642	-1.473676
O	-1.760624	-1.050508	-1.443010
O	-0.089769	-1.501635	0.304957
O	-1.206876	0.699796	0.207698
H	1.414780	-1.332284	0.403266
H	-2.250821	0.570412	0.303599
C	-4.239759	-0.574778	1.387176
N	-3.773859	0.194334	0.232975
C	-4.684131	1.265962	-0.167423
H	-3.529218	-1.382568	1.592695
H	-5.240840	-1.012513	1.231811
H	-4.286063	0.077765	2.268485
H	-3.589756	-0.436036	-0.555597
H	-4.291648	1.761033	-1.062105
H	-4.751613	2.010370	0.636258
H	-5.703721	0.902032	-0.382486
C	3.062659	-1.654145	1.696319
N	2.497971	-1.167102	0.424610
C	3.082030	-1.793572	-0.780589
H	2.562513	-1.146195	2.526321
H	4.138625	-1.449396	1.738943
H	2.896616	-2.732915	1.787608
H	2.594571	-0.089786	0.347843
H	2.562761	-1.387227	-1.653367
H	2.929500	-2.877358	-0.741854
H	4.155081	-1.577433	-0.837990
C	1.857861	2.344222	1.182345
N	2.412088	1.598942	0.048936
C	3.487140	2.318182	-0.632406
H	0.976295	1.819029	1.565361
H	1.550432	3.367594	0.904151
H	2.606759	2.423163	1.982492
H	1.651387	1.385556	-0.613558
H	3.809408	1.754946	-1.515945
H	4.349287	2.428817	0.039341
H	3.184510	3.328905	-0.959409

Isomers III -C3

S	-0.617268	-0.434784	-0.707218
O	0.340176	-0.427063	-1.816111
O	-0.803444	0.885253	-0.059851
O	-2.010278	-0.858948	-1.322218
O	-0.267348	-1.481353	0.314086
H	-2.785938	-0.577196	-0.670332

H	1.287115	-1.383026	0.445957
C	-3.528772	-0.396602	1.676683
N	-3.945947	-0.104793	0.297748
C	-4.164598	1.329174	0.062371
H	-3.407133	-1.477756	1.800589
H	-4.250255	-0.023133	2.422727
H	-2.555615	0.075672	1.850205
H	-4.799693	-0.621110	0.084037
H	-4.529704	1.479764	-0.959305
H	-3.202393	1.843546	0.162072
H	-4.887273	1.767856	0.770880
C	2.901208	-1.506479	1.802945
N	2.348632	-1.152655	0.482594
C	3.024813	-1.808447	-0.657249
H	2.329291	-0.989348	2.579228
H	3.953962	-1.208093	1.866135
H	2.822962	-2.587306	1.962786
H	2.357024	-0.066453	0.350279
H	2.485423	-1.529595	-1.566877
H	2.988626	-2.895971	-0.530573
H	4.070082	-1.483162	-0.711701
C	2.461160	2.478322	1.247274
N	2.084294	1.600654	0.139160
C	2.578840	2.077782	-1.156532
H	1.993528	2.127437	2.174855
H	2.154751	3.526639	1.083158
H	3.551329	2.467338	1.383790
H	1.054550	1.532619	0.088633
H	2.159895	1.446721	-1.947190
H	3.675681	2.017629	-1.186144
H	2.292470	3.125427	-1.354451

Isomers III -C4

S	-1.994898	-0.559685	-0.222074
O	-1.594768	-1.967426	-0.288249
O	-1.611644	0.286395	-1.348847
O	-3.632785	-0.565100	-0.297301
O	-1.661097	0.066233	1.090952
H	-3.927010	-1.347975	0.200855
H	-0.711053	1.338101	0.806406
C	2.127814	-3.075515	-0.260229
N	1.349965	-2.022430	0.387196
C	1.408750	-2.100194	1.845326
H	1.981535	-3.029639	-1.345721

H	1.853560	-4.091552	0.081418
H	3.198207	-2.934031	-0.053500
H	0.366072	-2.100918	0.100353
H	0.708280	-1.375121	2.275559
H	2.423841	-1.863733	2.196447
H	1.145650	-3.101019	2.236860
C	1.717559	0.686277	-2.116999
N	1.979085	0.702908	-0.671415
C	3.363939	1.061691	-0.358982
H	0.685478	0.363577	-2.292091
H	2.403843	0.011083	-2.656785
H	1.845549	1.694963	-2.533526
H	1.785432	-0.254940	-0.293358
H	3.535553	0.983569	0.721500
H	3.567778	2.096978	-0.665673
H	4.096108	0.412639	-0.870981
C	-0.600043	3.143032	-0.246902
N	0.006460	2.109922	0.620306
C	0.506733	2.625518	1.909712
H	-1.015236	2.643752	-1.126369
H	0.160950	3.874871	-0.540329
H	-1.405906	3.654199	0.291485
H	0.829521	1.591079	0.081680
H	0.930210	1.796595	2.485013
H	-0.315123	3.072011	2.479787
H	1.280399	3.382016	1.737560

Isomers III -C5

S	-0.115782	1.737719	-0.117172
O	1.000139	1.433216	-1.017733
O	-1.416048	1.954273	-0.749695
O	-0.187654	0.791029	1.031955
O	0.321565	3.174498	0.535408
H	0.038895	-0.738661	0.441077
H	-0.500047	3.598703	0.839857
C	-4.087296	-0.919233	-0.983318
N	-2.991341	-0.713622	-0.043316
C	-3.444175	-0.712483	1.343302
H	-3.719205	-0.821667	-2.011853
H	-4.923551	-0.204155	-0.850950
H	-4.498611	-1.932002	-0.864171
H	-2.544180	0.186282	-0.243812
H	-2.610910	-0.435419	1.999196
H	-3.793060	-1.716800	1.625702

H	-4.279078	-0.008665	1.533690
C	3.471123	-0.189190	1.261019
N	2.979753	-0.542360	-0.074839
C	4.043108	-1.001910	-0.968779
H	2.646753	0.228020	1.850442
H	4.285182	0.555117	1.229211
H	3.852507	-1.085464	1.768564
H	2.513922	0.284199	-0.477488
H	3.634210	-1.180341	-1.969870
H	4.463758	-1.945018	-0.595203
H	4.869525	-0.275288	-1.057270
C	0.152877	-2.752317	0.987821
N	0.447213	-1.643957	0.057501
C	-0.063060	-1.865168	-1.317424
H	0.539381	-2.500401	1.979865
H	0.628594	-3.672650	0.632511
H	-0.931146	-2.894704	1.043527
H	1.508962	-1.405695	0.018845
H	0.215134	-1.000539	-1.927338
H	-1.154669	-1.943348	-1.270612
H	0.381288	-2.777749	-1.729809

Isomers III -C6

S	0.046272	1.856994	-0.092204
O	1.025195	1.268212	-1.013446
O	-0.925607	2.778698	-0.652188
O	-0.564049	0.813314	0.789206
O	0.994875	2.745544	0.919474
H	-0.115738	-0.673555	0.292979
H	0.433362	3.471019	1.244354
C	3.439661	-0.469824	1.298498
N	2.931382	-0.753189	-0.046692
C	3.951132	-1.316381	-0.931942
H	2.665086	0.040558	1.881905
H	4.337897	0.171337	1.286641
H	3.701419	-1.408954	1.804263
H	2.557076	0.117303	-0.448818
H	3.541556	-1.433594	-1.941744
H	4.257000	-2.306041	-0.567212
H	4.855361	-0.686164	-0.996369
C	-0.116222	-2.666777	0.924014
N	0.280365	-1.610712	-0.030893
C	-0.176299	-1.864403	-1.417951
H	0.235531	-2.395625	1.923917

H	0.327809	-3.622957	0.626802
H	-1.208296	-2.746805	0.926947
H	1.351572	-1.443534	-0.022636
H	0.142941	-1.023544	-2.040183
H	-1.269209	-1.932734	-1.414767
H	0.265109	-2.797164	-1.786001
C	-3.824882	-0.276935	-1.095989
N	-3.110767	-0.742463	0.089534
C	-4.018364	-1.086273	1.177742
H	-3.108995	0.085023	-1.843112
H	-4.536631	0.544714	-0.885067
H	-4.395892	-1.105777	-1.538382
H	-2.470330	-0.006288	0.399137
H	-3.445241	-1.333701	2.079911
H	-4.614121	-1.968506	0.903187
H	-4.727952	-0.274960	1.435269

Isomers III -C7

S	-0.425322	-0.819525	0.051876
O	0.419613	-0.830960	-1.188496
O	-1.607951	-1.737027	-0.125395
O	0.390912	-1.262155	1.228568
O	-0.937649	0.585644	0.293583
H	1.936795	-1.361136	0.777253
H	-2.560048	0.589758	0.172072
C	-4.347464	0.010387	1.159925
N	-3.453129	0.021677	-0.008664
C	-4.082325	0.400733	-1.284415
H	-3.768487	-0.287715	2.038611
H	-5.160267	-0.706998	1.001438
H	-4.772499	1.007248	1.323793
H	-2.881148	-0.914298	-0.101707
H	-3.319564	0.374137	-2.067889
H	-4.501683	1.411095	-1.216930
H	-4.881155	-0.306841	-1.532470
C	1.675065	3.400010	1.076831
N	1.596931	2.326098	0.098113
C	1.590587	2.813458	-1.274321
H	1.589928	2.986087	2.088741
H	0.887803	4.172713	0.953840
H	2.646503	3.910424	1.000588
H	0.744165	1.777114	0.254297
H	1.412180	1.973842	-1.956036
H	2.563945	3.262943	-1.521808

H	0.814546	3.582878	-1.466689
C	3.692583	-0.317949	0.169069
N	2.679214	-1.379468	-0.001758
C	3.205359	-2.744007	-0.184911
H	3.166226	0.647532	0.245536
H	4.365178	-0.311200	-0.696348
H	4.275585	-0.509685	1.076930
H	1.968408	-1.132527	-0.766642
H	2.361581	-3.432027	-0.289687
H	3.805631	-3.031651	0.684975
H	3.828196	-2.787269	-1.084863

Isomers III -C8

S	0.512670	0.270726	-0.181504
O	-0.219342	0.971211	-1.280366
O	1.057946	-1.028899	-0.583342
O	1.725455	1.213538	0.186515
O	-0.347161	0.191719	1.037249
H	2.632833	0.629155	0.186274
H	-1.765617	1.219997	0.823220
C	4.756423	-0.015369	-0.934766
N	3.776982	-0.343736	0.102636
C	4.374412	-0.676756	1.396938
H	4.233300	0.181560	-1.876353
H	5.489104	-0.823452	-1.096399
H	5.303469	0.891038	-0.647108
H	3.164399	-1.103164	-0.214624
H	3.581983	-0.947017	2.102821
H	4.903639	0.199707	1.791029
H	5.091899	-1.511375	1.329768
C	-3.632867	1.311712	-0.152013
N	-2.261214	1.805950	0.100195
C	-2.147050	3.242589	0.423444
H	-3.579239	0.217354	-0.258701
H	-4.025928	1.777616	-1.061654
H	-4.276719	1.570672	0.696082
H	-1.576803	1.557141	-0.698971
H	-1.090128	3.484300	0.567816
H	-2.707052	3.466415	1.337288
H	-2.547662	3.836194	-0.404370
C	-3.191791	-2.757562	1.054631
N	-2.591005	-1.855136	0.080937
C	-2.288112	-2.518583	-1.184135
H	-3.317658	-2.242077	2.014670

H	-2.597879	-3.676338	1.232784
H	-4.186504	-3.072212	0.707744
H	-1.728285	-1.461949	0.466297
H	-1.732695	-1.834442	-1.834808
H	-3.223623	-2.799879	-1.688727
H	-1.682166	-3.437135	-1.061438

Isomers III -C9

S	-0.324584	2.058620	-0.236055
O	-0.042271	3.446855	-0.537211
O	0.551620	1.359601	0.706034
O	-1.760867	1.772117	0.033884
O	-0.001732	1.229136	-1.663075
H	-1.866076	0.356661	0.779602
H	-0.204362	1.854228	-2.380590
C	-1.149465	-0.817676	2.375082
N	-1.913038	-0.662720	1.116771
C	-3.326569	-1.079550	1.215737
H	-0.138241	-0.439799	2.206943
H	-1.123905	-1.873866	2.665109
H	-1.625725	-0.231936	3.168420
H	-1.416540	-1.202041	0.302656
H	-3.819175	-0.904691	0.254904
H	-3.833822	-0.492654	1.988603
H	-3.387844	-2.143259	1.470331
C	0.404841	-2.767738	-0.867558
N	-0.658659	-1.778612	-1.092974
C	-1.634093	-2.209877	-2.098868
H	1.190639	-2.320160	-0.242852
H	0.860631	-3.107950	-1.813659
H	-0.011683	-3.649134	-0.361447
H	-0.239366	-0.895301	-1.402572
H	-2.357105	-1.406824	-2.284532
H	-2.177711	-3.091668	-1.734767
H	-1.162193	-2.480299	-3.059122
C	3.607211	-0.708928	1.669745
N	2.829710	-0.643803	0.440057
C	3.669636	-0.476823	-0.738837
H	2.934323	-0.751471	2.535059
H	4.291074	0.152424	1.810729
H	4.221159	-1.621168	1.676838
H	2.167809	0.135294	0.494428
H	3.039601	-0.330027	-1.624360
H	4.276778	-1.379821	-0.898647

H 4.365619 0.383382 -0.670038

Isomers III -C10

S -0.549408 -0.763145 -1.150777
O -0.590693 0.695240 -1.357896
O -1.588044 -1.510996 -1.835667
O 0.822637 -1.332669 -1.337253
O -0.781380 -0.969376 0.462219
H 1.560085 -1.478637 -0.068099
H -1.626650 -0.379081 0.687216
C -4.081226 -0.059357 0.262951
N -2.855958 0.624169 0.694747
C -3.040761 1.470058 1.873805
H -3.863430 -0.639827 -0.639712
H -4.905790 0.643413 0.056962
H -4.407029 -0.749400 1.051251
H -2.486709 1.179795 -0.082910
H -2.102801 1.986989 2.106856
H -3.312517 0.844596 2.733553
H -3.833762 2.225458 1.739003
C 1.468998 3.215626 0.616647
N 1.861590 2.032452 -0.137048
C 2.825799 2.337493 -1.188143
H 0.690730 2.952058 1.343953
H 1.081281 4.037965 -0.017572
H 2.330316 3.610495 1.174837
H 1.028874 1.610945 -0.566062
H 3.009492 1.439253 -1.789153
H 3.780342 2.656543 -0.744094
H 2.492493 3.142571 -1.872236
C 2.009399 -3.009601 1.333651
N 1.863680 -1.578366 0.992493
C 3.033374 -0.725701 1.306242
H 1.089550 -3.530230 1.053554
H 2.196534 -3.128096 2.406296
H 2.848578 -3.426001 0.768616
H 1.001438 -1.202732 1.420012
H 2.796059 0.301003 0.980456
H 3.900523 -1.103354 0.754994
H 3.244089 -0.759880 2.381217

$(H_2SO_4)_2[(CH_3)_2NH]$

Isomer IV -A1

S 2.270930 -0.097096 0.000700

O	3.690261	0.018143	0.104306
O	1.496809	1.111411	-0.308667
O	1.953308	-1.186738	-1.087864
O	1.723096	-0.707681	1.344859
H	0.960807	-1.400804	-1.104535
H	0.704390	-0.763098	1.314177
S	-1.541547	-1.181110	-0.067978
O	-0.608835	-1.795818	-1.027211
O	-2.388335	-0.114248	-0.611749
O	-2.620606	-2.320397	0.304836
O	-0.875596	-0.779400	1.196025
H	-2.135089	-3.148066	0.478170
H	-0.019066	1.745454	-0.090628
C	-1.269967	2.654936	1.309275
N	-0.987084	2.163563	-0.062516
C	-1.099370	3.194003	-1.123447
H	-1.197420	1.808018	1.996310
H	-2.279716	3.074400	1.343013
H	-0.537941	3.421910	1.578401
H	-1.626626	1.349779	-0.281884
H	-0.869219	2.730956	-2.086370
H	-0.387243	4.000144	-0.925023
H	-2.118222	3.591847	-1.138820

Isomer IV -A2

S	1.528128	-1.182570	-0.058695
O	0.865722	-0.781883	1.196697
O	0.616925	-1.727012	-1.078390
O	2.425169	-0.135014	-0.580680
O	2.469632	-2.404529	0.417143
H	1.655272	1.337316	-0.285349
H	2.871920	-2.801516	-0.377454
S	-2.272479	-0.088370	0.001767
O	-1.483775	1.117256	-0.281164
O	-3.691354	0.039061	0.095104
O	-1.956566	-1.163524	-1.101375
O	-1.744818	-0.725484	1.341923
H	-0.963472	-1.370581	-1.129267
H	-0.729392	-0.788801	1.322711
C	1.295215	2.639622	1.306772
N	1.011000	2.147216	-0.064589
C	1.112907	3.179139	-1.124928
H	1.227490	1.792149	1.993577
H	0.560215	3.403155	1.577552

H	2.303154	3.063584	1.338252
H	0.044074	1.725659	-0.087823
H	0.882899	2.715455	-2.087599
H	2.128728	3.584643	-1.142991
H	0.395523	3.979919	-0.923770

Isomer IV -A3

S	2.178345	-0.519977	-0.089093
O	3.589744	-0.652524	0.081391
O	1.510122	-0.523376	1.343427
O	1.672931	0.647769	-0.826818
O	1.639169	-1.818132	-0.779681
H	0.506634	1.704660	-0.383411
H	0.621127	-1.802503	-0.828423
S	-1.824682	-0.878458	-0.007244
O	-2.649158	0.070563	-0.740402
O	-0.970221	-1.767802	-0.795651
O	-1.059622	-0.187831	1.090623
O	-2.817116	-1.915690	0.737155
H	0.492229	-0.474058	1.266482
H	-3.612290	-1.420043	1.004609
C	0.200086	3.216628	1.021596
N	-0.307433	2.267011	-0.000021
C	-1.065033	2.897331	-1.111334
H	0.753131	2.654823	1.779105
H	-0.641436	3.739677	1.484805
H	0.867172	3.938186	0.541595
H	-0.881240	1.522812	0.460101
H	-1.443600	2.106052	-1.762134
H	-0.398572	3.566707	-1.662745
H	-1.906840	3.462006	-0.700369

Isomer IV -A4

S	-2.304216	-0.077190	0.029404
O	-3.724179	-0.010370	0.154166
O	-1.561869	1.162740	-0.208471
O	-1.718379	-0.786642	1.301737
O	-1.984585	-1.080923	-1.156145
H	-0.695590	-0.788088	1.271650
H	-1.009770	-1.309599	-1.164240
S	1.729969	-1.220809	0.063953
O	2.561983	-2.352503	0.390484
O	0.858219	-0.710393	1.148941
O	2.367821	-0.109594	-0.660808

O	0.629413	-1.819920	-1.070846
H	1.594205	1.301456	-0.310956
H	0.754053	-2.786168	-1.070197
C	1.338726	2.646149	1.272088
N	0.985539	2.141899	-0.078495
C	1.092147	3.152166	-1.158814
H	1.251155	1.817572	1.979143
H	0.654804	3.453417	1.550330
H	2.367949	3.016596	1.261473
H	0.008524	1.756515	-0.061686
H	0.810336	2.684487	-2.105672
H	2.123249	3.512495	-1.218842
H	0.417639	3.986965	-0.947348

Isomer IV -A5

S	2.304220	-0.077252	0.029394
O	3.724187	-0.010488	0.154132
O	1.561926	1.162698	-0.208554
O	1.984530	-1.081043	-1.156084
O	1.718372	-0.786597	1.301779
H	1.009703	-1.309673	-1.164177
H	0.695586	-0.788069	1.271670
S	-1.730019	-1.220757	0.063962
O	-0.858226	-0.710393	1.148937
O	-2.562067	-2.352430	0.390483
O	-2.367854	-0.109507	-0.660765
O	-0.629506	-1.819887	-1.070865
H	-1.594161	1.301489	-0.310941
H	-0.754265	-2.786119	-1.070292
C	-1.092050	3.152174	-1.158819
N	-0.985456	2.141911	-0.078495
C	-1.338599	2.646184	1.272090
H	-0.810254	2.684483	-2.105676
H	-0.417524	3.986962	-0.947362
H	-2.123145	3.512523	-1.218844
H	-0.008453	1.756493	-0.061706
H	-1.251033	1.817614	1.979154
H	-2.367813	3.016657	1.261496
H	-0.654650	3.453438	1.550310

Isomer IV -A6

S	-0.642324	1.022644	-0.062155
O	0.332955	1.674261	-0.937793
O	-1.992582	1.603152	-0.097210

O	-0.690596	-0.466886	-0.300245
O	-0.175532	1.210488	1.443198
H	-2.387653	-1.020843	-0.165858
H	0.756518	0.827523	1.506065
S	2.758317	-0.515556	0.066568
O	2.215585	0.064590	1.296591
O	4.046934	-1.128258	0.089586
O	1.725736	-1.589323	-0.470298
O	2.773174	0.599746	-1.049937
H	0.790559	-1.210627	-0.408933
H	1.884995	1.081373	-1.044969
C	-4.208875	-1.004709	-1.214784
N	-3.367471	-0.662201	-0.044515
C	-3.912610	-1.077059	1.270259
H	-3.708204	-0.651783	-2.120143
H	-5.182197	-0.515101	-1.117795
H	-4.344906	-2.089039	-1.265307
H	-3.122405	0.373246	-0.037785
H	-3.210724	-0.769165	2.049918
H	-4.036764	-2.163771	1.290133
H	-4.879281	-0.591387	1.431680

Isomer IV -A7

S	-2.258550	-0.265119	-0.012555
O	-3.681823	-0.308886	0.083358
O	-1.630037	1.023453	-0.344092
O	-1.656204	-0.771458	1.351625
O	-1.801387	-1.327462	-1.071075
H	-0.639032	-0.766523	1.307827
H	1.508881	1.485099	-0.293967
S	1.669300	-1.256008	0.017310
O	0.949217	-0.664627	1.166253
O	2.600140	-2.318138	0.297972
O	0.799581	-1.451671	-1.159018
O	2.622038	0.076899	-0.401191
H	-0.782635	-1.368827	-1.127887
H	3.265695	-0.231221	-1.063911
C	0.950383	2.656708	1.323874
N	0.760712	2.175923	-0.070195
C	0.737555	3.251998	-1.092632
H	0.987229	1.784407	1.980728
H	0.109136	3.299993	1.596057
H	1.887898	3.216327	1.392079
H	-0.154690	1.638506	-0.128483

H 0.581506 2.799869 -2.075519
H 1.686377 3.796479 -1.076602
H -0.087191 3.935354 -0.873144

Isomer IV -A8

S -2.305567 -0.354462 -0.054737
O -3.725848 -0.442058 0.060418
O -1.735125 0.917685 -0.501410
O -1.649455 -0.741114 1.335195
O -1.801704 -1.500465 -1.021236
H -0.719920 -1.096363 1.152349
H -0.826986 -1.659561 -0.829020
S 1.783622 -0.974962 0.024652
O 1.978040 -0.611832 -1.369577
O 0.519117 -1.750403 0.242958
O 2.974209 -1.975848 0.466892
O 1.927444 0.116623 1.001131
H 3.026331 -2.686553 -0.198448
H 1.182366 1.494414 0.457417
C 0.350508 3.332538 1.039118
N 0.576291 2.259266 0.041446
C 1.184843 2.716423 -1.235135
H -0.104955 2.893886 1.930876
H -0.319969 4.087407 0.618024
H 1.308068 3.791231 1.301792
H -0.335106 1.774717 -0.163954
H 1.365696 1.837257 -1.859486
H 2.134293 3.216196 -1.021676
H 0.501745 3.408832 -1.735494

Isomer IV -A9

S -2.096611 -0.902793 -0.141399
O -2.180390 -2.023794 -1.048415
O -0.807176 -0.828684 0.628990
O -2.438185 0.428368 -0.675733
O -3.230108 -1.106249 1.008149
H -1.267311 1.476050 -0.339466
H -3.305899 -2.065605 1.161058
S 2.445848 -0.487765 -0.133611
O 3.674058 -0.965766 -0.698959
O 1.907186 0.794454 -0.565383
O 1.386310 -1.603470 -0.224728
O 2.646329 -0.261995 1.461250
H 0.411028 -1.292923 0.105119

H	3.145902	-1.024875	1.807901
C	-0.480915	3.307902	-1.001562
N	-0.462832	2.136547	-0.093114
C	-0.554476	2.478358	1.348507
H	-0.408930	2.954039	-2.033271
H	0.367201	3.961250	-0.776375
H	-1.418500	3.854853	-0.866525
H	0.413261	1.585538	-0.252812
H	-0.544503	1.546399	1.919240
H	-1.489869	3.014832	1.532022
H	0.297799	3.103065	1.632023

Isomer IV -A10

S	-2.172707	-0.855809	0.081333
O	-2.492542	0.476341	-0.466801
O	-3.200976	-1.505014	0.859062
O	-1.932642	-1.751669	-1.260131
O	-0.835261	-0.815160	0.762727
H	-2.223705	-2.656607	-1.046956
H	0.416842	1.598710	-0.285541
S	2.406875	-0.499615	-0.143498
O	1.896224	0.782857	-0.607191
O	3.609578	-1.030315	-0.716619
O	2.640455	-0.229057	1.438724
O	1.315000	-1.587298	-0.180507
H	3.107874	-1.001660	1.808155
H	0.360727	-1.252075	0.190416
C	-0.459277	2.565167	1.324449
N	-0.451082	2.154530	-0.102040
C	-0.529850	3.280818	-1.062493
H	-0.407192	1.662878	1.939030
H	-1.386870	3.103992	1.538032
H	0.402858	3.207938	1.526154
H	-1.270320	1.484389	-0.268871
H	-0.518400	2.878075	-2.078621
H	0.326151	3.947454	-0.921045
H	-1.461006	3.830604	-0.897659

Isomer IV -A11

S	-1.932096	-0.626070	0.046572
O	-1.336158	-0.645257	-1.297845
O	-1.263024	-1.508098	1.022044
O	-2.137085	0.745437	0.565238
O	-3.394712	-1.252442	-0.201091

H	-0.835186	1.705498	0.275393
H	-3.778346	-1.469116	0.668729
S	2.059981	-0.899546	-0.074407
O	3.265846	-0.141955	0.097737
O	2.056053	-2.290829	-0.428716
O	1.196703	-0.654533	1.236763
O	1.216268	-0.077945	-1.194969
H	0.288943	-1.119928	1.186426
H	0.294830	-0.486801	-1.323676
C	-0.309398	3.269755	-1.011267
N	0.047386	2.232447	-0.010952
C	0.748156	2.747793	1.194514
H	-0.826447	2.787505	-1.844991
H	0.599770	3.761532	-1.369046
H	-0.971453	4.004870	-0.545139
H	0.635512	1.498777	-0.467079
H	0.985111	1.900193	1.842186
H	0.093176	3.452170	1.714951
H	1.672554	3.247720	0.891499

Isomer IV -B1

S	-2.445995	-0.487557	-0.133558
O	-3.674106	-0.965293	-0.699349
O	-1.907336	0.794933	-0.564530
O	-2.646703	-0.262706	1.461388
O	-1.386391	-1.603160	-0.225177
H	-3.146269	-1.025814	1.807548
H	-0.411133	-1.292756	0.104867
S	2.096576	-0.902967	-0.141435
O	2.180511	-2.024182	-1.048168
O	0.807109	-0.828792	0.628891
O	3.230033	-1.106025	1.008223
O	2.438057	0.428091	-0.676092
H	3.305908	-2.065334	1.161385
H	1.267401	1.475923	-0.339625
C	0.555153	2.478395	1.348492
N	0.463074	2.136542	-0.093091
C	0.481086	3.307863	-1.001585
H	0.545231	1.546459	1.919265
H	-0.296973	3.103209	1.632220
H	1.490657	3.014769	1.531731
H	-0.413146	1.585659	-0.252530
H	0.408743	2.953978	-2.033260
H	1.418801	3.854664	-0.866839

H -0.366857 3.961360 -0.776174

Isomer IV -B2

S -2.406936 -0.499491 -0.143474
O -1.896278 0.783135 -0.606734
O -3.609562 -1.030061 -0.716881
O -1.315018 -1.587123 -0.180684
O -2.640704 -0.229403 1.438795
H -0.360757 -1.251952 0.190346
H -3.108157 -1.002120 1.807945
S 2.172661 -0.855910 0.081317
O 3.200884 -1.505141 0.859086
O 0.835216 -0.815138 0.762713
O 2.492580 0.476188 -0.466892
O 1.932539 -1.751821 -1.260100
H 1.270438 1.484339 -0.268908
H 2.223464 -2.656788 -1.046857
C 0.459670 2.565265 1.324447
N 0.451264 2.154543 -0.102017
C 0.529979 3.280768 -1.062548
H 0.407620 1.663018 1.939091
H -0.402405 3.208094 1.526226
H 1.387319 3.104056 1.537874
H -0.416722 1.598770 -0.285369
H 0.518364 2.877966 -2.078650
H 1.461194 3.830501 -0.897872
H -0.325959 3.947469 -0.921023

$(H_2SO_4)_2[(CH_3)_2NH]_2$

Isomer V -A1

S -1.028134 -1.889849 -0.377479
O 0.253465 -2.615237 -0.303209
O -1.050614 -0.847450 -1.421987
O -2.136294 -2.995593 -0.815922
O -1.541741 -1.427088 0.917706
H -1.834672 -3.395152 -1.652200
H 1.594411 -1.736554 0.278837
S 1.018416 1.932143 -0.510744
O -0.309404 2.574187 -0.677537
O 2.165299 2.773602 -0.746935
O 1.042468 1.185160 0.791700
O 1.118273 0.782611 -1.649206
H -1.887260 0.277395 0.807086
H 0.299444 0.210093 -1.609419

C	-3.444868	1.351477	-0.035019
N	-2.171781	1.284530	0.720528
C	-2.222378	1.896304	2.068152
H	-3.295673	0.856692	-0.998263
H	-3.716574	2.399231	-0.194221
H	-4.234773	0.841305	0.524997
H	-1.403824	1.777300	0.149623
H	-1.227637	1.819684	2.514846
H	-2.956406	1.370521	2.686944
H	-2.499943	2.950574	1.976085
C	2.585175	-1.584776	2.097822
N	2.324735	-1.118568	0.717326
C	3.528010	-1.051662	-0.145675
H	1.635387	-1.625250	2.637962
H	3.262854	-0.884597	2.595663
H	3.035088	-2.582473	2.074848
H	1.858102	-0.143274	0.752468
H	3.225823	-0.670553	-1.124509
H	3.969788	-2.048519	-0.242918
H	4.253428	-0.364467	0.300198

Isomer V -A2

S	2.692779	-0.079094	-0.101248
O	3.018681	0.974026	-1.052550
O	1.602545	0.251668	0.844867
O	2.507411	-1.417658	-0.704515
O	3.966355	-0.220792	0.915011
H	0.992109	-2.009166	-0.337886
H	4.762568	-0.293558	0.358444
S	-2.693031	0.079306	0.101814
O	-3.020620	-0.973473	1.052876
O	-2.506711	1.417690	0.705107
O	-1.602563	-0.252416	-0.843737
O	-3.965912	0.222146	-0.915211
H	0.622732	1.507718	0.339415
H	-4.762577	0.293259	-0.359078
C	-0.075123	-2.582422	1.364039
N	0.008421	-2.322471	-0.096629
C	-0.376425	-3.479407	-0.937827
H	0.318584	-1.705914	1.884266
H	0.530912	-3.460605	1.607559
H	-1.120941	-2.741043	1.640135
H	-0.622587	-1.508097	-0.339952
H	-0.293626	-3.194330	-1.989957

H	-1.409798	-3.760308	-0.714542
H	0.292517	-4.320111	-0.730558
C	0.377608	3.479237	0.936613
N	-0.008069	2.322135	0.096001
C	0.074771	2.581534	-1.364788
H	0.295042	3.194599	1.988877
H	-0.291017	4.320164	0.729230
H	1.411035	3.759538	0.712837
H	-0.991727	2.009167	0.337837
H	-0.319390	1.704924	-1.884506
H	1.120475	2.739798	-1.641496
H	-0.531226	3.459749	-1.608293

Isomer V -A3

S	1.311420	-1.799437	-0.361052
O	1.756796	-1.697265	1.023963
O	0.063201	-2.562025	-0.552009
O	1.314984	-0.498508	-1.078180
O	2.453956	-2.609715	-1.191828
H	-0.213076	0.329051	-1.470571
H	2.549204	-3.484276	-0.772848
S	-1.309496	1.846208	-0.372348
O	-1.087651	0.789816	-1.588592
O	-2.625786	2.384619	-0.612727
O	-1.178217	1.017933	0.871132
O	-0.190873	2.819074	-0.439335
H	-1.824025	-0.413450	0.716434
H	1.135417	2.220316	0.207271
C	3.232889	2.298283	0.019308
N	1.998023	1.668657	0.539483
C	1.959386	1.510580	2.013250
H	3.162752	2.362918	-1.069745
H	4.101280	1.693019	0.297251
H	3.332269	3.303370	0.439960
H	1.865471	0.739270	0.073851
H	0.984945	1.095723	2.280009
H	2.086890	2.491882	2.480679
H	2.754651	0.830073	2.329874
C	-2.379098	-2.059945	1.896446
N	-2.164814	-1.426497	0.575743
C	-3.358900	-1.415637	-0.303493
H	-1.435628	-2.042795	2.449018
H	-2.703991	-3.096591	1.762119
H	-3.141489	-1.501852	2.448273

H	-1.359113	-1.905447	0.093984
H	-3.094649	-0.905080	-1.233123
H	-4.166005	-0.867417	0.191519
H	-3.675071	-2.443305	-0.508589

Isomer V -A4

S	-2.178491	0.510809	-0.565323
O	-1.731232	1.907326	-0.800304
O	-3.561478	0.226327	-0.849909
O	-1.350673	-0.406738	-1.632593
O	-1.698154	0.051025	0.776530
H	-0.403327	-0.117200	-1.633532
H	-1.022750	-1.400361	0.787720
S	2.300274	-0.555599	-0.411708
O	1.838254	0.089709	0.830966
O	3.672773	-0.326752	-0.803197
O	1.829596	-1.948140	-0.527232
O	1.377374	0.300701	-1.551330
H	-0.480766	2.228335	0.139790
H	1.832459	0.187523	-2.405375
C	-1.396657	-3.340571	0.103198
N	-0.534572	-2.354304	0.797906
C	-0.197124	-2.712271	2.194836
H	-1.601764	-2.966993	-0.903264
H	-2.338542	-3.446731	0.649825
H	-0.883686	-4.305968	0.052465
H	0.363866	-2.220516	0.257312
H	0.462110	-1.939684	2.599496
H	0.317638	-3.677882	2.213599
H	-1.114501	-2.769300	2.788621
C	1.209034	3.476808	0.217268
N	0.358157	2.406354	0.786449
C	-0.146542	2.687138	2.151336
H	1.536177	3.167513	-0.778591
H	2.083144	3.632995	0.856896
H	0.629779	4.402195	0.145252
H	0.905113	1.506937	0.798009
H	-0.795809	1.859247	2.447035
H	-0.722452	3.617486	2.139483
H	0.695757	2.780402	2.844003

Isomer V -A5

S	2.729146	-0.000564	-0.003588
O	2.257365	1.036178	-0.943950

O	4.151682	0.003868	0.280306
O	1.811469	-0.178520	1.125546
O	2.511701	-1.442497	-0.892030
H	-0.742673	1.836797	0.328101
H	3.399461	-1.837155	-0.934783
S	-2.580669	0.055145	0.082806
O	-3.049526	-1.061384	0.892749
O	-2.267428	1.281464	0.844360
O	-1.501765	-0.279503	-0.876594
O	-3.798169	0.452632	-0.936248
H	-0.587538	-1.522140	-0.321437
H	-4.606270	0.514104	-0.395712
C	-0.468811	-3.496606	-0.933617
N	-0.023546	-2.386024	-0.057475
C	-0.186347	-2.658327	1.396038
H	-0.320208	-3.204821	-1.976586
H	-1.531109	-3.683477	-0.754134
H	0.111662	-4.397211	-0.711212
H	0.969875	-2.144080	-0.264982
H	0.260412	-1.825297	1.942871
H	0.331106	-3.589659	1.647026
H	-1.253633	-2.731503	1.620332
C	-0.318253	3.255576	-1.114602
N	0.101237	2.382970	0.008129
C	0.663563	3.113675	1.170179
H	-0.733682	2.624332	-1.904396
H	0.551083	3.800771	-1.493251
H	-1.082013	3.956616	-0.765541
H	0.844096	1.716833	-0.348940
H	0.980431	2.378263	1.914034
H	-0.102022	3.772302	1.591043
H	1.528017	3.699594	0.844385

Isomer V -B1

S	-1.016519	-1.895490	-0.377078
O	-1.047521	-0.853760	-1.422081
O	-1.532509	-1.436071	0.918319
O	-2.116899	-3.009356	-0.814226
O	0.270473	-2.611267	-0.303624
H	-1.815065	-3.404483	-1.652526
H	1.606385	-1.726210	0.280492
S	1.005390	1.936803	-0.511437
O	2.147998	2.784276	-0.747028
O	1.032849	1.189618	0.790879

O	-0.325700	2.571985	-0.678218
O	1.111608	0.788348	-1.650174
H	-1.415465	1.768913	0.149164
H	0.296199	0.210846	-1.610421
C	-2.232439	1.883589	2.068428
N	-2.180187	1.271950	0.720800
C	-3.454440	1.332078	-0.033298
H	-1.236850	1.811869	2.514035
H	-2.963262	1.354305	2.688023
H	-2.515219	2.936491	1.976515
H	-1.889969	0.266454	0.807114
H	-3.303964	0.837307	-0.996346
H	-3.731459	2.378368	-0.192988
H	-4.241210	0.818507	0.528022
C	2.599208	-1.568160	2.097996
N	2.333607	-1.103879	0.717881
C	3.534925	-1.029867	-0.147277
H	1.650721	-1.613579	2.640030
H	3.274058	-0.864178	2.594316
H	3.054454	-2.563427	2.074538
H	1.860671	-0.131636	0.753246
H	3.228691	-0.650682	-1.125600
H	3.982465	-2.024089	-0.245237
H	4.257030	-0.338313	0.297225

Isomer V -B2

S	1.014544	1.932666	-0.511786
O	-0.314170	2.572964	-0.677782
O	2.160235	2.775569	-0.748760
O	1.040313	1.186086	0.790946
O	1.115288	0.783124	-1.649944
H	1.859764	-0.139403	0.753218
H	0.297140	0.209493	-1.609915
S	-1.025626	-1.891128	-0.377288
O	-1.051718	-0.848386	-1.421474
O	0.258321	-2.612253	-0.303606
O	-1.540658	-1.430386	0.918055
O	-2.130236	-3.000270	-0.815922
H	-1.888477	0.274033	0.807523
H	-1.828143	-3.397732	-1.653024
C	3.530491	-1.044905	-0.146483
N	2.328491	-1.113845	0.718181
C	2.591613	-1.579015	2.098470
H	3.226158	-0.664919	-1.125086

H	3.974209	-2.040891	-0.243841
H	4.255057	-0.355973	0.298078
H	1.598931	-1.733069	0.280588
H	1.642686	-1.620802	2.640021
H	3.268844	-0.877507	2.595046
H	3.043157	-2.575974	2.075343
C	-3.448174	1.346575	-0.032782
N	-2.174183	1.280834	0.721263
C	-2.223740	1.892630	2.068953
H	-3.299873	0.851285	-0.995903
H	-3.720664	2.394075	-0.192322
H	-4.237135	0.836327	0.528491
H	-1.407355	1.774417	0.149608
H	-1.228470	1.816615	2.514565
H	-2.956828	1.366447	2.688509
H	-2.501973	2.946742	1.977108

Isomer V -B3

S	-1.024985	-1.928709	-0.511613
O	0.300831	-2.574959	-0.677563
O	-2.174442	-2.766172	-0.749420
O	-1.047797	-1.182597	0.791416
O	-1.120054	-0.778069	-1.649314
H	-1.857074	0.148878	0.752907
H	-0.298784	-0.209038	-1.609500
S	1.034667	1.886131	-0.378159
O	1.055831	0.842620	-1.421661
O	-0.245028	2.614990	-0.306573
O	1.545046	1.423031	0.918220
O	2.146577	2.988246	-0.815909
H	1.885006	-0.282865	0.807936
H	1.848899	3.385891	-1.654514
C	3.439989	-1.361688	-0.032963
N	2.166526	-1.290868	0.721643
C	2.214267	-1.902731	2.069315
H	3.292954	-0.866393	-0.996275
H	3.708595	-2.410271	-0.191982
H	4.231015	-0.853949	0.527681
H	1.397543	-1.781270	0.150209
H	1.219481	-1.822928	2.515360
H	2.949565	-1.379259	2.688566
H	2.488513	-2.957892	1.977498
C	-3.524387	1.063164	-0.144150
N	-2.320410	1.125907	0.718252

C	-2.578561	1.592783	2.098913
H	-3.223989	0.680937	-1.123102
H	-3.962690	2.061563	-0.241267
H	-4.251976	0.378562	0.302172
H	-1.588458	1.741383	0.279214
H	-1.628333	1.630331	2.638503
H	-3.258031	0.894583	2.597101
H	-3.025519	2.591822	2.076337

Isomer V -B4

S	-2.809544	0.007931	0.274632
O	-2.928526	1.129456	1.194517
O	-2.970300	-1.329489	0.832162
O	-3.969902	0.201035	-0.869489
O	-1.584285	0.097602	-0.594446
H	-4.822924	0.219342	-0.399234
H	-0.727729	-1.351438	-0.388996
S	2.829030	-0.075235	0.234579
O	2.928927	-1.092147	1.271382
O	2.453504	1.267469	0.737584
O	4.316220	0.097384	-0.418158
O	2.026867	-0.462375	-0.947418
H	4.944971	0.136155	0.324907
H	-0.565801	1.409598	-0.315408
C	0.420935	2.717342	-1.588966
N	0.120712	2.208706	-0.228421
C	-0.427222	3.231019	0.696747
H	0.851436	1.899833	-2.173192
H	1.143456	3.535842	-1.518381
H	-0.501862	3.070802	-2.058448
H	1.019668	1.806845	0.176946
H	-0.660125	2.751859	1.650224
H	-1.348608	3.644990	0.277935
H	0.315649	4.021687	0.839230
C	0.020720	-2.750945	0.980530
N	-0.033444	-2.148141	-0.376671
C	-0.396542	-3.103702	-1.448655
H	0.403698	-2.003133	1.678606
H	0.705618	-3.603756	0.966787
H	-0.987671	-3.057206	1.269827
H	0.879657	-1.665560	-0.598596
H	-0.418192	-2.572031	-2.403711
H	-1.386667	-3.517977	-1.237655
H	0.345384	-3.906696	-1.489562

Isomer V -B5

S	-0.980461	-1.917003	-0.371983
O	-1.015494	-0.872426	-1.401338
O	-1.549828	-1.481779	0.918460
O	-2.000796	-3.027168	-0.982172
O	0.312760	-2.610441	-0.221578
H	-1.956081	-3.811602	-0.406000
H	1.888900	-0.093956	0.745860
S	0.961965	1.963393	-0.490096
O	-0.382635	2.572198	-0.644926
O	2.085496	2.839590	-0.711909
O	1.006952	1.193764	0.798140
O	1.092317	0.838630	-1.650454
H	-1.925920	0.215034	0.801963
H	0.297780	0.235348	-1.610542
C	-3.486215	1.258385	-0.074209
N	-2.228916	1.216678	0.709252
C	-2.321179	1.827587	2.054872
H	-3.308001	0.760802	-1.031058
H	-3.771437	2.300649	-0.245428
H	-4.279830	0.738620	0.471624
H	-1.460912	1.728434	0.155370
H	-1.335828	1.769148	2.524490
H	-3.059484	1.289027	2.657387
H	-2.615408	2.876725	1.955934
C	3.532803	-0.969878	-0.233283
N	2.384463	-1.054372	0.700995
C	2.741234	-1.485043	2.070945
H	3.162461	-0.617177	-1.199120
H	3.997808	-1.955388	-0.337809
H	4.261532	-0.252776	0.156560
H	1.647762	-1.699989	0.315434
H	1.829424	-1.531453	2.672604
H	3.434353	-0.761220	2.510231
H	3.209956	-2.473859	2.040298

Isomer V -B6

S	2.300128	-0.554846	-0.412077
O	3.672336	-0.324322	-0.803560
O	1.830931	-1.947852	-0.527830
O	1.837393	0.089542	0.830869
O	1.376369	0.300749	-1.551375
H	0.365879	-2.220327	0.257755

H	1.832024	0.189039	-2.405313
S	-2.179167	0.510010	-0.564997
O	-3.562226	0.226609	-0.850238
O	-1.699807	0.049725	0.776955
O	-1.351428	-0.408027	-1.632062
O	-1.730832	1.906217	-0.799832
H	-0.404228	-0.118078	-1.633456
H	-0.480618	2.227766	0.139728
C	-1.394272	-3.340904	0.103189
N	-0.532786	-2.354220	0.798030
C	-0.195732	-2.711829	2.195158
H	-1.598875	-2.967719	-0.903525
H	-2.336463	-3.447023	0.649306
H	-0.881090	-4.306227	0.053130
H	-1.021436	-1.400595	0.787595
H	0.463335	-1.939091	2.599808
H	0.319088	-3.677406	2.214265
H	-1.113275	-2.768795	2.788696
C	1.208222	3.477679	0.217164
N	0.358341	2.406461	0.786273
C	-0.146522	2.686731	2.151230
H	1.536140	3.168546	-0.778499
H	2.081898	3.635056	0.857109
H	0.627984	4.402421	0.144656
H	0.905959	1.507364	0.797692
H	-0.794945	1.858195	2.447000
H	-0.723430	3.616467	2.139409
H	0.695743	2.780893	2.843823

Isomer V -B7

S	-1.935884	1.023700	-0.603763
O	-1.191897	2.289290	-0.811564
O	-3.338911	1.039448	-0.933210
O	-1.287869	-0.064061	-1.615361
O	-1.624342	0.492994	0.770211
H	-0.287047	0.003480	-1.589717
H	-1.361054	-1.012366	0.785760
S	2.087509	-0.898192	-0.481426
O	1.413252	-0.063751	-1.497169
O	3.483863	-1.168314	-0.736649
O	1.721321	-0.512487	0.895376
O	1.311657	-2.395039	-0.575236
H	1.169821	1.164494	0.864543
H	1.584807	-2.795729	-1.419873

C	0.542171	2.694342	2.126991
N	0.944339	2.187320	0.794224
C	2.099872	2.892116	0.188952
H	-0.336965	2.131525	2.450909
H	0.288766	3.755689	2.047377
H	1.364631	2.561772	2.836949
H	0.100659	2.251780	0.133217
H	2.311678	2.433188	-0.780347
H	2.973023	2.797675	0.841848
H	1.847836	3.948108	0.053775
C	-0.846695	-2.521426	2.165962
N	-1.190688	-2.088277	0.790933
C	-2.388483	-2.746055	0.214297
H	0.071291	-2.008663	2.465055
H	-0.689671	-3.604549	2.188076
H	-1.665174	-2.252711	2.840256
H	-0.368033	-2.245735	0.177021
H	-2.560502	-2.330178	-0.782048
H	-3.252742	-2.529872	0.848759
H	-2.230652	-3.827863	0.156962

Isomer V -B8

S	0.487247	-1.747308	-0.144914
O	-0.649610	-2.605511	-0.500692
O	0.163496	-0.923707	1.060558
O	1.796390	-2.409197	-0.018966
O	0.743814	-0.727561	-1.350101
H	2.693573	-0.907281	0.125347
H	0.082933	0.076523	-1.349964
S	-0.735582	2.107947	-0.067182
O	-0.730552	1.318403	-1.339307
O	-0.549374	3.525403	-0.231568
O	-1.876819	1.681703	0.779121
O	0.594891	1.590837	0.751477
H	-2.336481	0.153536	0.398967
H	0.376067	0.632971	1.013379
C	3.810429	0.270793	1.450648
N	3.065297	0.086814	0.179415
C	3.849810	0.375083	-1.049419
H	3.143331	0.025986	2.280934
H	4.140152	1.310166	1.532588
H	4.674487	-0.399419	1.459912
H	2.218052	0.696821	0.190656
H	3.203548	0.191162	-1.910832

H	4.717147	-0.290042	-1.083357
H	4.176898	1.418624	-1.035390
C	-3.422403	-1.316293	1.399440
N	-2.771700	-0.798275	0.171862
C	-3.685498	-0.627791	-0.984387
H	-2.658333	-1.417209	2.174315
H	-3.873166	-2.291735	1.193489
H	-4.190572	-0.609217	1.725677
H	-1.996686	-1.454625	-0.092454
H	-3.111196	-0.209451	-1.814954
H	-4.485021	0.066397	-0.710106
H	-4.108468	-1.596922	-1.265476

Isomer V -B9

S	-0.487455	-2.130751	-0.063211
O	-0.560425	-1.056475	-1.287913
O	0.114019	-3.336534	-0.593058
O	0.318510	-1.453366	0.997571
O	-1.902738	-2.258085	0.351960
H	1.786204	-1.110357	0.635162
H	-2.479683	-0.760040	0.365375
S	0.507006	2.304223	-0.329164
O	-0.915278	2.166579	0.021195
O	0.876889	3.564900	-0.934268
O	1.335147	2.230873	1.105586
O	1.035009	1.088504	-1.007766
H	1.407656	3.151368	1.414489
H	0.032563	-0.267530	-1.120650
C	-3.676911	0.381938	-0.908677
N	-2.846762	0.248186	0.312948
C	-3.554331	0.581253	1.570400
H	-3.067421	0.085741	-1.765984
H	-4.001822	1.420758	-1.020193
H	-4.545951	-0.278005	-0.829461
H	-2.010422	0.878359	0.213096
H	-2.864116	0.442307	2.406623
H	-4.413080	-0.085948	1.690922
H	-3.891577	1.621796	1.539888
C	3.617636	-0.323011	1.361847
N	2.714543	-0.699830	0.252119
C	3.296217	-1.652389	-0.725085
H	3.096867	0.392247	2.002961
H	4.528038	0.135017	0.961848
H	3.877116	-1.218900	1.933893

H	2.363159	0.150514	-0.243526
H	2.535232	-1.897035	-1.470825
H	3.584391	-2.568901	-0.202465
H	4.170844	-1.203335	-1.205990