

## Supporting Information

### Propionamide Participating in H<sub>2</sub>SO<sub>4</sub>-based New Particle Formation: A Theory Study

Xianwei Zhao<sup>1</sup>, Yunfeng Li<sup>1,3</sup>, Chenpeng Zuo<sup>1</sup>, Yanhui Sun<sup>5</sup>, Fei Xu<sup>1,4,\*</sup>, Alexey B. Nadykto<sup>2,\*</sup>, Lin Du<sup>1</sup>, Yisheng Xu<sup>3</sup>, Qingzhu Zhang<sup>1</sup>, Wenxing Wang<sup>1</sup>

<sup>1</sup>Environment Research Institute, Shandong University, Qingdao 266237, P. R. China

<sup>2</sup>Department of Applied Mathematics, Moscow State University of Technology “Stankin”, Vadkovsky 1, Moscow 127055, Russia

<sup>3</sup> Chinese Research Institute Environmental Science, State Key Laboratory Environmental Criteria & Risk Assessment, Beijing 100012, P. R. China

<sup>4</sup>Shenzhen Research Institute of Shandong University, Shenzhen 518057, P. R. China

<sup>5</sup>College of Environment and Safety Engineering, Qingdao University of Science & Technology, Qingdao 266042, P. R. China

\*Corresponding authors. E-mail: xufei@sdu.edu.cn.

\*Corresponding authors. E-mail: a.nadykto@stankin.ru.

Fax: 86-532-5863 1986; 7495-9729521.

#### Boundary condition

**Figure S1.** The ratio between the monomer collision rate and the cluster total evaporation rate for (PA)<sub>m</sub>(SA)<sub>n</sub> (m = 0–3 and n = 0–3) at 298.15 K.

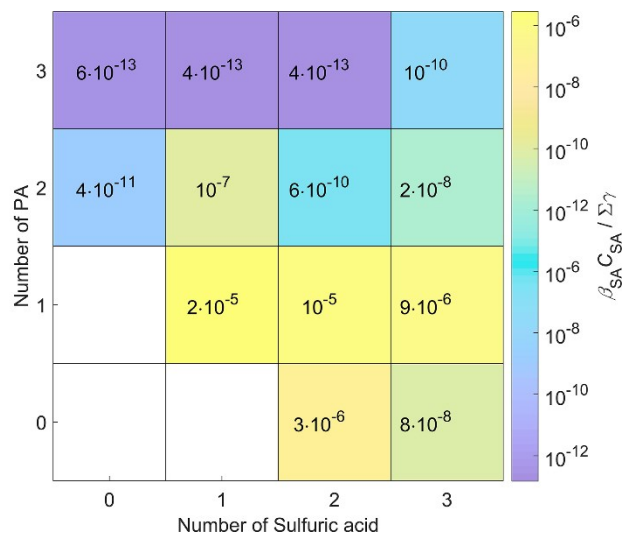
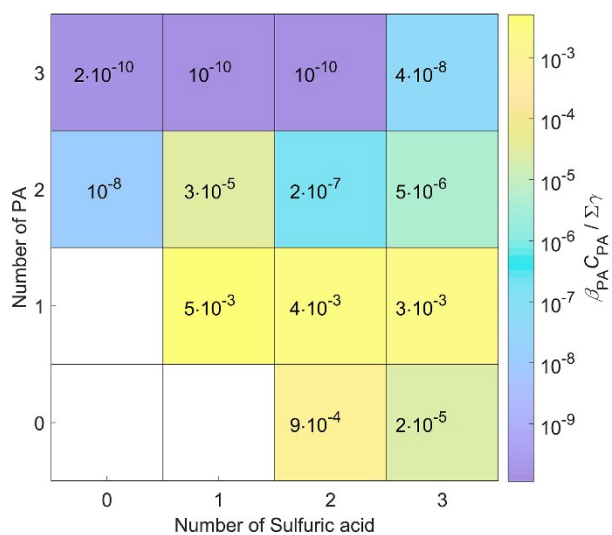
**Figure S2.** Main clustering pathways (left panel) and actual Gibbs free energy surface for the formation of (DMA)<sub>m</sub>(SA)<sub>n</sub> clusters (right panel) at 298.15 K, [H<sub>2</sub>SO<sub>4</sub>] = 10<sup>6</sup> cm<sup>-3</sup>, and [DMA] = 10 ppt.

**Figure S3.** Evaporation rates for (DMA)<sub>m</sub>(SA)<sub>n</sub> clusters at 298.15 K.

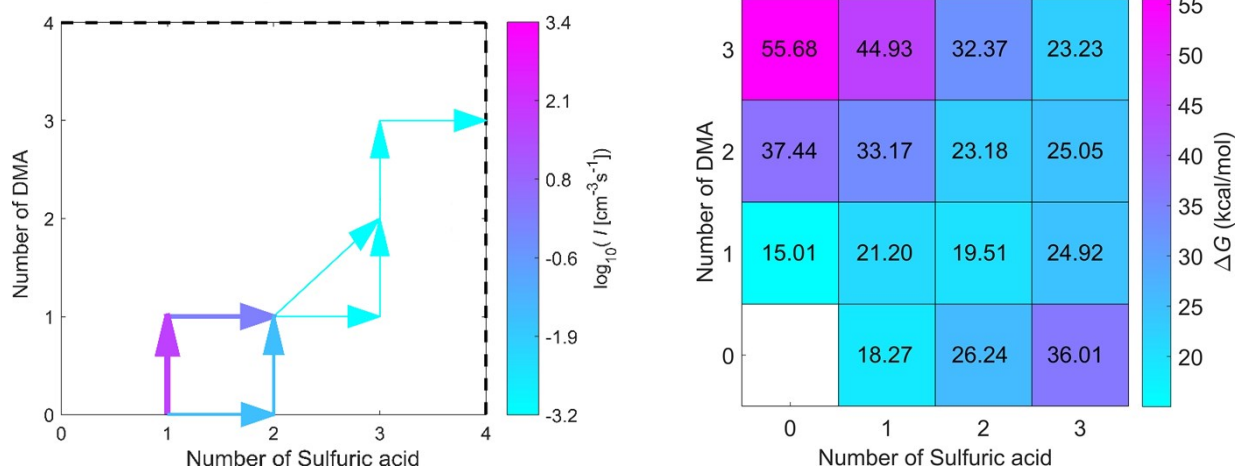
**Table S1.** Evaporation coefficients (s<sup>-1</sup>) for all evaporation pathways of the (PA)<sub>m</sub>(SA)<sub>n</sub> (m = 0–3 and n = 0–3) clusters under simulation at 298.15 K.

**Table S2.** Coordinates of all optimized clusters.

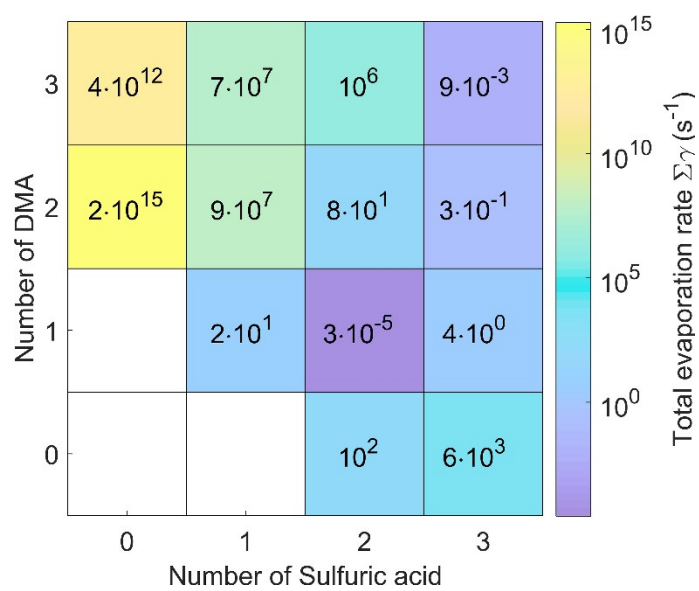
**Boundary condition.** Boundary conditions require that the growing clusters could be sufficiently stable and the clusters should be more likely to grow than evaporate. For  $(\text{PA})_m(\text{SA})_n$  ( $m = 0-3$  and  $n = 0-3$ ) clusters, clusters with roughly equal numbers of SA and PA molecules or the number of SA molecules is one more than that of PA molecules have lower evaporation rates and higher concentrations in the simulations. Therefore, we suppose that  $(\text{PA})_4(\text{SA})_4$  and  $(\text{PA})_3(\text{SA})_4$  clusters are stable enough and do not evaporate. In the ACDC simulation,  $(\text{PA})_4(\text{SA})_4$  and  $(\text{PA})_3(\text{SA})_4$  that can be formed by collisions between small clusters or evaporation of larger clusters in the simulation could leave the simulation box. Similarly, for  $(\text{DMA})_m(\text{SA})_n$  ( $m = 0-3$  and  $n = 0-3$ ) clusters,  $(\text{DMA})_4(\text{SA})_4$  and  $(\text{DMA})_3(\text{SA})_4$  could leave the simulation box. All other clusters crossing the box edge for  $\text{H}_2\text{SO}_4$ -PA and  $\text{H}_2\text{SO}_4$ -DMA system will be brought back to the simulation box by monomer evaporations.



**Figure S1.** The ratio between the monomer collision rate and the cluster total evaporation rate for  $(PA)_m(SA)_n$  ( $m = 0-3$  and  $n = 0-3$ ) at 298.15 K



**Figure S2.** Main clustering pathways (left panel) and actual Gibbs free energy surface for the formation of  $(\text{DMA})_m(\text{SA})_n$  clusters (right panel) at 298.15 K,  $[\text{H}_2\text{SO}_4] = 10^6 \text{ cm}^{-3}$ , and  $[\text{DMA}] = 10 \text{ ppt}$ .



**Figure S3.** Evaporation rates for (DMA)<sub>m</sub>(SA)<sub>n</sub> clusters at 298.15 K.

**Table S1.** Evaporation coefficients ( $s^{-1}$ ) for all evaporation pathways of the  $(PA)_m(SA)_n$  ( $m = 0-3$  and  $n = 0-3$ ) clusters under simulation at 298.15 K.

	Evaporation coefficients
$(SA)_2 \rightarrow SA + SA$	1.21E+02
$(SA)_3 \rightarrow (SA)_2 + SA$	5.53E+03
$(PA)(SA) \rightarrow PA + SA$	2.42E+01
$(PA)(SA)_2 \rightarrow (PA)(SA) + SA$	3.33E+01
$(PA)(SA)_2 \rightarrow (SA)_2 + PA$	3.14E+00
$(PA)(SA)_3 \rightarrow (PA)(SA)_2 + SA$	4.90E+01
$(PA)(SA)_3 \rightarrow (PA)(SA) + (SA)_2$	5.41E+00
$(PA)(SA)_3 \rightarrow (SA)_3 + PA$	2.66E-02
$(PA)_2 \rightarrow PA + PA$	1.21E+07
$(PA)_2(SA) \rightarrow (PA)_2 + SA$	4.49E-03
$(PA)_2(SA) \rightarrow (PA)(SA) + PA$	4.23E+03
$(PA)_2(SA)_2 \rightarrow (PA)_2(SA) + SA$	4.35E+03
$(PA)_2(SA)_2 \rightarrow (PA)_2 + (SA)_2$	6.21E-02
$(PA)_2(SA)_2 \rightarrow (PA)(SA)_2 + PA$	5.30E+05
$(PA)_2(SA)_2 \rightarrow (PA)(SA) + (PA)(SA)$	3.11E+05
$(PA)_2(SA)_3 \rightarrow (PA)_2(SA)_2 + SA$	1.25E+00
$(PA)_2(SA)_3 \rightarrow (PA)_2(SA) + (SA)_2$	1.54E+01
$(PA)_2(SA)_3 \rightarrow (PA)_2 + (SA)_3$	1.15E-05
$(PA)_2(SA)_3 \rightarrow (PA)(SA)_3 + PA$	1.31E+04
$(PA)_2(SA)_3 \rightarrow (PA)(SA)_2 + (PA)(SA)$	2.00E+04
$(PA)_3 \rightarrow (PA)_2 + PA$	8.61E+08
$(PA)_3(SA) \rightarrow (PA)_3 + SA$	6.53E-03
$(PA)_3(SA) \rightarrow (PA)_2(SA) + PA$	1.21E+09
$(PA)_3(SA) \rightarrow (PA)_2 + (PA)(SA)$	1.83E+05
$(PA)_3(SA)_2 \rightarrow (PA)_3(SA) + SA$	3.91E+01
$(PA)_3(SA)_2 \rightarrow (PA)_3 + (SA)_2$	7.04E-04
$(PA)_3(SA)_2 \rightarrow (PA)_2(SA)_2 + PA$	1.05E+07
$(PA)_3(SA)_2 \rightarrow (PA)_2(SA) + (PA)(SA)$	1.38E+09
$(PA)_3(SA)_2 \rightarrow (PA)(SA)_2 + (PA)_2$	1.79E+05
$(PA)_3(SA)_3 \rightarrow (PA)_3(SA)_2 + SA$	9.33E-02
$(PA)_3(SA)_3 \rightarrow (PA)_3(SA) + (SA)_2$	9.21E-03
$(PA)_3(SA)_3 \rightarrow (PA)_3 + (SA)_3$	8.70E-09
$(PA)_3(SA)_3 \rightarrow (PA)_2(SA)_3 + PA$	7.67E+05
$(PA)_3(SA)_3 \rightarrow (PA)_2(SA)_2 + (PA)(SA)$	2.64E+04
$(PA)_3(SA)_3 \rightarrow (PA)_2(SA) + (PA)(SA)_2$	2.97E+06
$(PA)_3(SA)_3 \rightarrow (PA)_2 + (PA)(SA)_3$	2.94E+02

**Table S2.** Coordinates of all optimized clusters.

H <sub>2</sub> SO <sub>4</sub>			
S	0.00026100	-0.14164400	0.00000000
O	0.00053600	-0.85706900	-1.22344500
O	0.00732500	-0.85615700	1.22399000
O	1.13855000	0.94120200	-0.00339100
O	-1.14639600	0.93205300	0.00260700
H	-2.00285400	0.48510900	0.00387500
H	1.99855000	0.50096700	-0.00196100
(H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub>			
S	-2.07325700	0.07047100	0.11993300
O	-3.33837400	0.66690900	0.41607800
O	-1.12697600	-0.22456900	1.18397200
O	-2.29025300	-1.35668300	-0.58679500
H	-3.04913600	-1.28785100	-1.19746200
O	-1.38385400	0.93792600	-0.98661100
H	-0.40663900	0.67919800	-1.08309300
S	2.07325500	-0.07050200	-0.11992000
O	1.12695700	0.22445400	-1.18396700
O	3.33837400	-0.66694900	-0.41605100
O	2.29026200	1.35675200	0.58660400
H	3.04913400	1.28797200	1.19728800
O	1.38387000	-0.93779900	0.98675300
H	0.40662000	-0.67915600	1.08318900
(H <sub>2</sub> SO <sub>4</sub> ) <sub>3</sub>			
S	0.00993600	0.51347300	0.08237400
O	-0.86511800	1.67228600	-0.38397500
H	-1.80503000	1.37223700	-0.56333800
O	0.53301800	-0.05835100	-1.24488500
H	1.44635500	-0.44618800	-1.12810200
O	-0.79907800	-0.46818500	0.74736600
O	1.09915900	1.05930100	0.83210900
S	-4.01039400	-0.24987000	-0.12508000
O	-4.23471200	0.37753100	1.29757000
H	-4.91583800	-0.11499500	1.77580100
O	-3.13467500	-1.48383400	0.15573600
H	-2.20478600	-1.20560200	0.38023100
O	-3.23966700	0.73743900	-0.82100200
O	-5.23956100	-0.69449700	-0.65154000
S	3.99100100	-0.39311200	-0.00978300
O	3.49815500	0.11716100	1.35755900
H	2.58009800	0.48810400	1.27835400
O	4.27730700	0.92596600	-0.81432300
H	5.12729900	1.30212100	-0.54777300
O	2.90285200	-1.00066300	-0.71515100
O	5.19272200	-1.09959400	0.19611700
PA			
C	1.91863600	0.12622500	-0.00022500
H	1.94858400	0.76094900	-0.88620000
H	2.82689700	-0.47273500	-0.00000200
H	1.94873800	0.76179400	0.88514000
C	0.69127600	-0.77547900	0.00029600

H	0.69267700	-1.43228500	-0.86941000
H	0.69275700	-1.43138700	0.87067400
C	-0.67053700	-0.10147500	-0.00000400
O	-1.69081500	-0.75244900	-0.00018500
N	-0.68479100	1.25839400	0.00001300
H	0.15243500	1.80938100	0.00065700
H	-1.57826900	1.71948200	0.00012400
(PA) <sub>2</sub>			
C	4.36650700	-0.66513000	0.00004300
H	4.14660800	-1.27035600	0.87641900
H	5.42643300	-0.41863600	0.00011900
H	4.14667400	-1.27003500	-0.87657400
C	3.52380800	0.59888400	0.00021600
H	3.74286800	1.21493600	0.87473500
H	3.74322700	1.21545400	-0.87384300
C	2.03416600	0.30147200	-0.00008200
O	1.61105400	-0.84614600	0.00000500
N	1.22235000	1.37250600	-0.00029200
H	1.60681900	2.29953100	-0.00054900
H	0.20830500	1.24629000	-0.00033400
C	-4.36651000	0.66511800	0.00007100
H	-4.14651800	1.27019900	0.87652500
H	-5.42643600	0.41862200	0.00023300
H	-4.14676700	1.27016900	-0.87646700
C	-3.52380500	-0.59889200	0.00000700
H	-3.74308000	-1.21527300	0.87424000
H	-3.74300700	-1.21513700	-0.87433900
C	-2.03416600	-0.30146900	0.00005600
O	-1.61106700	0.84615400	0.00018300
N	-1.22234000	-1.37249500	-0.00022000
H	-1.60680200	-2.29952300	0.00009000
H	-0.20829500	-1.24627000	-0.00005100
(PA) <sub>3</sub>			
C	-3.43221600	-3.78506800	0.16186100
H	-3.76739000	-3.48987600	1.15423000
H	-3.46150300	-4.87090100	0.09423300
H	-4.13417100	-3.36931800	-0.55673100
C	-2.02761000	-3.27144700	-0.10659600
H	-1.30937500	-3.68770500	0.60091400
H	-1.68937500	-3.57327900	-1.10028400
C	-1.93954700	-1.75791600	-0.04920800
O	-2.94948000	-1.05693200	-0.05391700
N	-0.70828200	-1.24124300	-0.01139300
H	0.13792200	-1.78944000	-0.00682200
H	1.43641600	1.12098600	0.02585900
C	-0.03392200	4.42290800	0.02005000
H	0.49860700	4.08049100	0.90496000
H	-0.05352300	5.51069600	0.02538800
H	0.52405500	4.08957900	-0.85259600
C	-1.44628600	3.86372600	-0.00318600
H	-2.01526900	4.20321100	0.86446600
H	-1.98950200	4.21119100	-0.88408800
C	-1.47111300	2.34540000	-0.01051000



O	-0.43207200	1.69189200	-0.00054300
N	-2.68010400	1.77370400	-0.02829100
H	-3.50439800	2.34738700	-0.03689200
H	-2.78533700	0.75063900	-0.03584600
C	4.89584800	-1.88915600	-0.07965000
H	4.49259400	-2.50445800	0.72088100
H	5.98240800	-1.94028200	-0.04871800
H	4.55235900	-2.31286300	-1.02086500
C	4.42405200	-0.45240900	0.06339900
H	4.76878500	-0.02223200	1.00638900
H	4.83266200	0.17613700	-0.73011600
C	2.90814100	-0.33633900	0.03306700
O	2.18778200	-1.31735700	0.01758500
N	2.43125200	0.92722500	0.03331800
H	3.06438600	1.70583500	0.04373700
H	-0.59434300	-0.23262000	-0.00390100
(PA)(H <sub>2</sub> SO <sub>4</sub> )			
C	-4.08624100	-0.99498300	-0.14885100
H	-3.95073900	-1.17721800	-1.21318700
H	-5.15195900	-0.98890200	0.06763300
H	-3.62189800	-1.81553700	0.39127900
C	-3.45835100	0.32963700	0.25734200
H	-3.91731700	1.16681200	-0.26903100
H	-3.60785200	0.50983500	1.32466200
C	-1.96525300	0.35692800	0.02976600
O	-1.31794600	-0.69532400	0.03069500
N	-1.39625400	1.54946600	-0.14005900
H	-1.95373200	2.38448900	-0.12679700
H	-0.38278700	1.62351300	-0.19837500
S	2.05536900	-0.01747900	-0.09535200
O	1.06064500	-1.06923700	-0.57426800
H	0.07120500	-0.86301300	-0.30016500
O	2.19947500	-0.31922700	1.45251700
H	2.79310000	-1.07083200	1.57445100
O	1.46117800	1.28117400	-0.14036100
O	3.30526200	-0.25804100	-0.71532900
(PA)(H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub>			
C	-6.02548600	-0.27570600	-0.30422600
H	-5.97884100	0.75098700	0.05571900
H	-7.00857900	-0.68434200	-0.07332700
H	-5.90256400	-0.26830700	-1.38813100
C	-4.94184800	-1.12403300	0.36424400
H	-5.07838000	-1.11672300	1.45013000
H	-4.98681300	-2.16314800	0.03403500
C	-3.57098100	-0.57342300	0.11347200
O	-3.41107300	0.67078100	0.31773700
N	-2.60242800	-1.35836200	-0.28713100
H	-2.79398600	-2.33809600	-0.42752000
H	-1.62271100	-1.03323400	-0.39161600
S	0.05057000	1.00389200	-0.12490500
O	1.13310100	1.63771100	-0.82689300
O	-0.00670300	-0.45423300	-0.36417200
O	0.26343200	1.18826000	1.42289900

H	1.13810300	0.79768100	1.64040600
O	-1.26071700	1.61186600	-0.35694600
H	-2.45338600	1.06440400	0.06817100
S	3.39227900	-0.57924300	0.12135700
O	4.61123500	-1.26519000	0.29962600
O	2.63386100	-0.11257400	1.25555600
O	3.67891100	0.64638700	-0.81071900
H	2.85613200	1.17593100	-0.90028400
O	2.44364100	-1.48003900	-0.73788800
H	1.50682100	-1.17578600	-0.63544400
(PA)(H <sub>2</sub> SO <sub>4</sub> ) <sub>3</sub>			
S	-3.21276000	-0.38209600	0.32686000
O	-2.50315300	0.02562900	-0.90253100
O	-4.45121800	0.25321300	0.63659300
O	-3.43883700	-1.93065200	0.27719200
H	-2.56092900	-2.40789900	0.08796800
O	-2.22725300	-0.14943600	1.53887200
H	-1.30602800	-0.50486100	1.30014600
S	3.38819400	-0.01694100	0.31926400
O	3.62241900	-1.39283900	-0.37586700
O	4.64085000	0.50408100	0.75617900
O	2.57256500	0.81098000	-0.60153300
H	2.09209300	2.25034100	-0.31579200
O	2.50459700	-0.33206700	1.58106200
H	1.57400700	-0.62820600	1.29426500
S	0.06207400	-2.07152300	-0.38131900
O	0.12717200	-1.05329600	0.73382300
O	-1.05924500	-2.99043100	-0.18790200
O	-0.23691300	-1.21873900	-1.70739500
H	-1.15858700	-0.84755800	-1.60292500
O	1.35870000	-2.68535400	-0.63171900
H	2.74637100	-1.89103600	-0.53016200
C	-2.11639800	3.80543500	-0.27476700
H	-2.35130600	3.51726300	-1.30645200
H	-2.67746300	4.71922100	-0.05640500
H	-2.49197500	3.02593900	0.39895900
C	-0.62600800	4.06196000	-0.08005800
H	-0.27138600	4.88456200	-0.71852200
H	-0.40471100	4.38485800	0.94764100
C	0.28147800	2.90749400	-0.35339500
O	1.55038600	3.11557400	-0.17777400
N	-0.17211300	1.74608600	-0.75373400
H	-1.17235800	1.53694600	-0.81867200
H	0.47195000	0.96414900	-0.90348800
(PA) <sub>2</sub> (H <sub>2</sub> SO <sub>4</sub> )			
C	3.94673700	-2.84770800	-0.38840800
H	3.17821400	-3.24017100	0.27911800
H	4.78561000	-3.54419000	-0.39723400
H	3.52195400	-2.79057400	-1.38967800
C	4.40503900	-1.46693500	0.06491700
H	4.81068600	-1.49573000	1.07938400
H	5.20560900	-1.10023000	-0.58642300
C	3.29136600	-0.44182800	-0.00725600

O	2.38088700	-0.58009500	-0.82876900
N	3.37535300	0.59829400	0.82671500
H	4.12755500	0.65871800	1.49076700
H	2.68362800	1.34531500	0.78450100
S	0.00000500	1.69830700	0.00006100
O	-1.19303800	2.42374000	-0.32453000
O	1.19312700	2.42362400	0.32467800
O	-0.26458900	0.74446600	1.19145000
H	-1.14036800	0.22736400	1.04673500
O	0.26444800	0.74442100	-1.19133000
H	1.14041700	0.22764700	-1.04698800
C	-3.94689800	-2.84765500	0.38866100
H	-3.17810700	-3.24015600	-0.27852500
H	-4.78576800	-3.54414700	0.39722900
H	-3.52249100	-2.79045400	1.39008700
C	-4.40503500	-1.46694900	-0.06502300
H	-4.81034700	-1.49592900	-1.07962300
H	-5.20580400	-1.10007900	0.58597000
C	-3.29131700	-0.44190000	0.00710100
O	-2.38041200	-0.58051300	0.82808400
N	-3.37552300	0.59845100	-0.82658500
H	-4.12859400	0.65971900	-1.48957600
H	-2.68382000	1.34548600	-0.78423400
(PA) <sub>2</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub>			
C	-6.20959600	0.35113900	-1.61354600
H	-6.33322200	1.30948500	-1.11248700
H	-7.15559200	0.08092900	-2.07648400
H	-5.46024300	0.47163600	-2.39098100
C	-5.78088900	-0.72635800	-0.62737300
H	-6.52336700	-0.86645200	0.15768700
H	-5.67506000	-1.68549800	-1.14002000
C	-4.43650500	-0.43784100	-0.00683600
O	-3.57280600	0.15915600	-0.66571400
N	-4.22458500	-0.86863900	1.23193300
H	-4.94818600	-1.35736900	1.72816500
H	-3.31144000	-0.75166400	1.66728900
S	-0.58985100	-0.17769600	0.94420900
O	-1.24090300	0.69495400	-0.13034700
H	-2.26413100	0.43949000	-0.30488500
O	-0.37768700	-1.54919200	0.28161700
H	0.48012100	-1.58093800	-0.26201800
O	-1.50684900	-0.37501300	2.02103200
O	0.68858800	0.40953600	1.24196000
S	3.11712500	-1.57738000	-0.35259900
O	3.99338500	-0.47767500	-0.91681400
H	3.59424600	0.50415600	-0.73249500
O	2.88673100	-1.19493200	1.13879300
H	2.15957600	-0.53803600	1.24243400
O	3.79497000	-2.81165100	-0.39144300
O	1.81490800	-1.49389100	-1.00941600
C	1.78307300	3.62454600	1.17087400
H	1.68682100	2.82329800	1.90002600
H	1.26510000	4.50362500	1.54764000

H	2.83853600	3.85994200	1.06174900
C	1.18662000	3.19847500	-0.16081400
H	0.12996100	2.94847100	-0.06132900
H	1.25681200	4.00428400	-0.89582200
C	1.89262300	2.00997000	-0.75650900
O	3.03690000	1.70693600	-0.39041100
N	1.25149400	1.34253200	-1.71903100
H	0.25831600	1.47419200	-1.81705000
H	1.62713300	0.45899300	-2.03632600
(PA) <sub>2</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>3</sub>			
C	-6.04344100	2.64863700	-0.58812500
H	-5.88836900	2.84764400	0.47348100
H	-6.84253000	3.29741000	-0.94654600
H	-5.12409700	2.89854000	-1.11640000
C	-6.40422400	1.18626000	-0.82014800
H	-7.32566600	0.91604000	-0.29867800
H	-6.57787900	1.00190100	-1.88569000
C	-5.29756300	0.24692000	-0.39912000
O	-4.11999100	0.64078900	-0.41096400
N	-5.64024100	-0.98900900	-0.04681100
H	-6.60432500	-1.27622700	-0.06423100
H	-4.91710400	-1.67594300	0.16145200
S	-1.92648100	-1.94049800	0.32790100
O	-2.04826000	-0.38916900	0.40771400
H	-2.97108000	-0.02748500	0.03797900
O	-1.38154300	-2.20889300	-1.09399000
H	-0.42022600	-1.88345700	-1.14271700
O	-3.24020200	-2.50464600	0.38530500
O	-0.94803100	-2.32334600	1.30256800
S	2.02111100	-1.76188200	-0.05740300
O	2.19679000	-0.90133700	1.11658400
H	3.54040500	-0.18592600	1.21966700
O	1.53020500	-3.16365400	0.45387000
H	0.69001700	-3.03486400	0.94197700
O	3.24893200	-2.03512000	-0.76555900
O	0.94664700	-1.22354300	-0.90951200
C	-1.97648400	2.78840100	0.99649400
H	-2.35693100	2.42404600	0.04025400
H	-2.69803100	3.50545900	1.38721200
H	-1.93716200	1.94719800	1.69162900
C	-0.61845900	3.46176500	0.84628700
H	-0.66712300	4.32946900	0.18333600
H	-0.24624600	3.83824400	1.80400500
C	0.46931400	2.59272900	0.30148000
O	1.58029900	3.19404400	0.04179800
N	0.30277000	1.32362400	0.10391800
H	-0.57114300	0.84874300	0.32857400
H	1.04522000	0.72543400	-0.26237400
S	4.50161800	0.99779500	-0.26236100
O	5.44833200	2.04410500	-0.24120900
O	4.40566500	0.34767400	1.13502600
O	3.13429100	1.30301000	-0.68614900
H	2.29156900	2.55245800	-0.27223100

O	5.02480900	-0.12515800	-1.19406900
H	4.40462400	-0.90393800	-1.16313400
(PA) <sub>3</sub> (H <sub>2</sub> SO <sub>4</sub> )			
C	-5.79895200	2.21916500	-1.29446900
H	-5.72899600	2.89082900	-0.43361400
H	-6.71038400	2.46608400	-1.84542100
H	-4.93716900	2.40585000	-1.93800700
C	-5.82164600	0.75339700	-0.85219500
H	-6.66924200	0.55519300	-0.18668700
H	-5.95148800	0.10398300	-1.72790600
C	-4.52374800	0.32443000	-0.18797000
O	-3.43574100	0.73690900	-0.63863600
N	-4.60962800	-0.51251900	0.85439100
H	-5.50605000	-0.83131100	1.18474900
H	-3.75745900	-0.87462900	1.28867400
S	-0.82939700	-0.97932200	0.99119300
O	-1.09306100	0.38125000	0.21591000
H	-2.08234000	0.46994800	-0.10269500
O	-0.71136700	-2.07362000	-0.12832700
H	0.24050000	-2.10022300	-0.58384600
O	-2.01033500	-1.30874200	1.79255300
O	0.45826100	-0.81623000	1.67187200
C	4.47592500	3.71643000	0.15781600
H	4.72512500	3.19392900	-0.77009500
H	5.40291800	4.12854400	0.57005100
H	3.81988600	4.55927200	-0.09038900
C	3.85353500	-2.51845900	-1.55650900
H	3.60035000	-3.03325500	-2.48361000
H	4.62977500	-3.07114700	-1.02137900
C	2.61027300	-2.33389600	-0.72809800
O	1.49777200	-2.21747000	-1.29466900
N	2.74880600	-2.27601600	0.60411700
H	3.67597700	-2.20563600	0.99435200
H	1.97418200	-1.91385800	1.16079100
C	3.80533500	2.76334100	1.15164800
H	4.48835900	1.93918000	1.38214500
H	3.60632600	3.28891100	2.09340400
H	4.22800600	-1.51454900	-1.78477300
C	2.48985600	2.17150100	0.63709000
H	1.97575900	1.62194200	1.43753800
H	1.80050000	2.96445100	0.32106300
C	2.67732300	1.17762700	-0.50702900
O	3.75108600	0.61488900	-0.72518800
N	1.56608300	0.95117200	-1.26547800
H	0.65546800	1.17858300	-0.88556300
H	1.59320000	0.13150000	-1.85891400
(PA) <sub>3</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub>			
C	-6.29416400	1.97035300	-1.37973600
H	-6.32352800	2.63935600	-0.52176500
H	-7.23879900	2.05120800	-1.91247700
H	-5.49195500	2.30064600	-2.03383400
C	-6.05981000	0.53350700	-0.93797400
H	-6.86210800	0.17979400	-0.29025100

H	-6.03825800	-0.13067200	-1.80534300
C	-4.73472200	0.35418200	-0.23462400
O	-3.79402600	1.11523400	-0.48244800
N	-4.63291500	-0.65921400	0.62454200
H	-5.42165400	-1.25568300	0.79785600
H	-3.74078800	-0.86427800	1.07270900
S	-0.95813200	-0.18107100	0.98998900
O	-1.54144000	1.19147600	0.57210200
H	-2.48738600	1.11846600	0.13765800
O	-0.69056500	-0.89975900	-0.33759100
H	0.03491400	-0.42315400	-0.91928800
O	-1.96682000	-0.94776200	1.66096300
O	0.25371900	0.11010000	1.68023600
S	2.42047300	0.24592600	-1.76510500
O	2.95543400	1.58869900	-2.01250900
H	3.27124400	2.37782700	-0.80492000
O	2.86672700	-0.05011500	-0.30808200
H	2.57003600	-0.98716900	-0.00906500
O	2.92142400	-0.77749000	-2.63562600
O	0.94469900	0.30448100	-1.75464600
C	3.01894800	1.50628900	2.77679300
H	2.52387800	0.58370500	2.48482600
H	3.06366500	1.55503100	3.86202900
H	4.03135700	1.50639300	2.38115400
C	2.23806000	2.71474500	2.24708500
H	1.21916600	2.71635900	2.62694200
H	2.72849700	3.64320600	2.54221500
C	2.21255700	2.68304400	0.75859400
O	3.33294400	2.77954000	0.14822900
N	1.08808300	2.55336900	0.11253500
H	0.23721200	2.32336800	0.60987600
H	1.08162500	2.40187100	-0.89071900
C	0.29803000	-3.81635700	1.94091600
H	1.26661800	-4.13619300	2.31876000
H	-0.47439200	-4.44602000	2.37737400
H	0.13596800	-2.79100100	2.26581400
C	0.25415100	-3.90526100	0.42474800
H	0.41344900	-4.92766800	0.07659000
H	-0.72105600	-3.58722100	0.04978400
C	1.28060100	-3.01207100	-0.23310900
O	2.01572100	-2.29279500	0.44441700
N	1.33672100	-3.04258900	-1.56958800
H	0.66223600	-3.57686500	-2.08725100
H	1.95493100	-2.41339200	-2.07574700
(PA) <sub>3</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>3</sub>			
C	-2.91860600	1.96674900	2.01248500
H	-2.69861800	0.90575100	2.11143600
H	-3.74815900	2.20328000	2.67416100
H	-2.04743600	2.53539300	2.32962800
C	-3.29739100	2.32270400	0.57297900
H	-4.13509500	1.73016600	0.21269000
H	-3.58090500	3.37594500	0.51548700
C	-2.14415600	2.15860300	-0.36241000

O	-1.07077300	2.79036300	-0.04513300
N	-2.25320100	1.42987700	-1.43147000
H	-3.11859000	0.87438500	-1.56346800
H	-1.48916000	1.34836400	-2.10656300
S	1.06442900	0.78991100	-1.94798100
O	1.08796400	1.85628900	-0.93499200
H	-0.22210400	2.46158200	-0.50943300
O	2.48920300	0.60329800	-2.47529000
H	3.04349700	-0.00029700	-1.85059000
O	0.19961300	1.10289900	-3.04589500
O	0.71427000	-0.49370800	-1.28361100
S	3.34734100	-2.17118500	-0.41992100
O	2.57688000	-2.02438400	0.84090800
H	1.25079900	-2.32240200	1.03840300
O	2.31559400	-2.67630400	-1.48617900
H	1.59872800	-2.01578300	-1.58104200
O	4.37855200	-3.13597600	-0.35781500
O	3.77624100	-0.83013700	-0.85719900
S	-0.45107600	-1.23179400	1.85013300
O	0.53244600	-0.50902500	2.63607200
H	0.86347900	1.04469000	2.48342100
O	-0.83340100	-0.33061700	0.64466100
H	-0.16696900	-0.40021000	-0.14935900
O	-1.66518800	-1.58518400	2.49327200
O	0.20505000	-2.44783900	1.23539500
C	4.01367300	2.97947800	0.04984400
H	4.87326900	2.48536200	0.50215400
H	4.34247700	3.95714800	-0.29188800
H	3.69029100	2.41147800	-0.82226500
C	2.87072800	3.13942300	1.03889400
H	3.17560800	3.70365300	1.92343600
H	2.03488000	3.67977300	0.59717100
C	2.30477400	1.85768200	1.54427900
O	1.22622600	1.94769000	2.24659200
N	2.88022400	0.71992000	1.32359700
H	3.63893100	0.63430000	0.65730600
H	2.47801000	-0.16753800	1.62198400
C	-7.13080900	-1.11531900	-1.14942200
H	-7.38220000	-0.17807600	-0.65614600
H	-8.00181100	-1.76569300	-1.11642000
H	-6.89701300	-0.89282600	-2.18715600
C	-5.94487700	-1.78303400	-0.47084800
H	-6.15746100	-2.01263500	0.57359900
H	-5.71230500	-2.73307000	-0.95793300
C	-4.68791200	-0.94614600	-0.55198800
O	-4.53656100	-0.10026300	-1.43084400
N	-3.75056900	-1.18305800	0.37781600
H	-3.86271100	-1.88344800	1.09123100
H	-2.83718500	-0.75504600	0.31244000
(MA) <sub>2</sub>			
N	-1.28495300	-0.67081400	0.05783400
H	-1.65269000	-1.46122500	0.57096800
H	-0.50756200	-0.29279100	0.58967000

C	-2.31314600	0.35126900	-0.10870900
H	-1.88363400	1.20503500	-0.63143600
H	-3.11867200	-0.03648000	-0.73052300
H	-2.75022900	0.71840500	0.82536100
N	1.43822200	0.75878900	0.18125000
H	0.98281700	1.12514600	-0.64572000
H	2.09614000	1.46223200	0.49082000
C	2.12694100	-0.49100900	-0.14213800
H	2.58312400	-0.89223000	0.76111400
H	1.39020200	-1.21100700	-0.49434800
H	2.90485200	-0.39446700	-0.90441700

(MA)<sub>3</sub>

N	0.87938800	-1.26606900	-0.42623700
H	0.15217900	-1.07840400	0.26236900
H	0.58200300	-2.07946700	-0.95036900
C	2.16135600	-1.52525600	0.22378900
H	2.92934300	-1.68647400	-0.53122800
H	2.45258900	-0.64891100	0.80099500
H	2.16106800	-2.38679300	0.89825400
N	0.12082900	1.74472700	-0.71613700
H	0.35370000	0.84007000	-1.11780500
H	0.26152600	2.44837000	-1.42919900
C	1.00650900	1.98104200	0.42118400
H	0.78345700	2.94857700	0.86906300
H	0.81765500	1.21709100	1.17626600
H	2.07321100	1.95459800	0.17757900
N	-1.74664000	-0.14217500	0.80375200
H	-2.35799400	-0.04939800	1.60394300
H	-1.43874300	0.78602800	0.52605300
C	-2.45001800	-0.75837400	-0.31861100
H	-1.78207000	-0.77468600	-1.17980300
H	-2.70446800	-1.78955700	-0.07536400
H	-3.36558000	-0.24088900	-0.61857500

(MA)(H<sub>2</sub>SO<sub>4</sub>)

S	-0.87927900	0.12549400	0.01780300
O	-1.60261000	1.33475500	-0.21168700
O	-1.97098600	-1.03211700	0.15077400
O	-0.04618400	-0.28211100	-1.14231900
O	-0.10472400	0.02198200	1.23271400
N	2.16900600	-0.72222300	-0.04281700
C	2.80263100	0.61331100	0.02306500
H	-2.77280900	-0.73550000	-0.29362800
H	1.22127900	-0.62520000	-0.65038000
H	1.80435700	-0.98341500	0.87409600
H	3.07714200	0.91949000	-0.98117100
H	3.67992100	0.59318200	0.66242100
H	2.06205400	1.29815600	0.42444500
H	2.79372700	-1.43900500	-0.39515900

(MA)(H<sub>2</sub>SO<sub>4</sub>)<sub>2</sub>



S	1.63540400	-0.78361200	-0.03130000
O	2.38602500	0.09878500	-0.90543400
O	0.99577500	-0.05814900	1.05619300
O	2.68892800	-1.69326500	0.71714500
O	0.74921600	-1.68301800	-0.74013700
H	1.58474400	1.58689500	-0.88450800
H	3.07804100	-2.31737300	0.09141200
S	-2.17037100	-0.10078000	-0.01189100
O	-1.57883300	-0.26612500	1.40880600
O	-3.56774400	0.03610100	0.09776200
O	-1.86766400	-1.44188100	-0.71268000
O	-1.42190800	0.93583700	-0.68468600
H	-0.58037500	-0.23200700	1.37412200
H	-0.88359800	-1.58427000	-0.79548200
N	0.88874400	2.34545000	-0.69220000
H	-0.02770400	1.85208200	-0.61369900
C	1.22376900	3.06082400	0.56315200
H	2.18246100	3.55574600	0.44787800
H	1.28010200	2.31953300	1.35283000
H	0.44820900	3.78792500	0.77985400
H	0.84341100	2.97236400	-1.49060900

(MA)(H<sub>2</sub>SO<sub>4</sub>)<sub>3</sub>

S	-1.16034400	1.88839900	-0.17379900
O	-1.96503800	1.24939100	0.86340900
O	0.22888500	2.01268200	0.23105000
O	-1.76205300	3.34364000	-0.21722200
O	-1.33387100	1.32740000	-1.49421300
H	0.98612100	0.18200000	1.79148100
H	-1.40414300	3.82587400	-0.97401500
S	-1.57025100	-1.78844600	-0.45930700
O	-2.75370500	-1.19277000	0.33920300
O	-0.35884500	-1.20724700	0.09328600
O	-1.74020700	-1.24182900	-1.88982500
O	-1.70695800	-3.18801800	-0.48726800
H	-2.59271200	-0.22780000	0.53303600
H	-1.57471800	-0.25952500	-1.89097400
N	0.21386500	0.23055800	2.49298800
H	-0.64634700	0.45628500	1.97590900
C	0.11759400	-1.05370700	3.22784500
H	1.06852400	-1.24850500	3.71232700
H	-0.09251000	-1.83156400	2.50213900
H	-0.67841800	-0.99469200	3.96264000
S	2.85818600	-0.14477200	-0.35723200

O	4.22047800	-0.30856000	-0.66838600
O	2.35085300	1.14172100	-1.04698600
O	2.44576700	-0.10173300	1.02593500
H	1.52388900	1.48868600	-0.61699500
O	2.07375500	-1.28845000	-1.04822400
H	1.15952100	-1.35007400	-0.68342200
H	0.41421200	1.01494200	3.10922300

(MA)<sub>2</sub>(H<sub>2</sub>SO<sub>4</sub>)

S	0.02252800	-0.56672600	0.08553300
O	-0.48276200	0.89009000	0.18714000
O	-1.10046100	-1.41466500	-0.16980800
O	0.84899100	-0.81881900	1.22543100
O	0.91227600	-0.56606000	-1.17282800
H	-1.45249900	0.95561400	-0.21594200
H	1.90521300	-0.36393900	-0.89526700
N	3.23696300	-0.01052900	-0.22183200
C	3.11540000	1.38855200	0.21138800
H	3.20027600	-0.62807200	0.58284500
H	3.10543900	2.03207100	-0.66505400
H	2.16636100	1.50258300	0.73071500
H	3.92231300	1.70221900	0.87326600
N	-2.90217200	0.78931900	-0.67031100
C	-3.67473600	0.47622600	0.54044500
H	-2.82835800	-0.03761300	-1.25417800
H	-3.69010400	1.34924400	1.18839300
H	-4.69987900	0.17517400	0.32574500
H	-3.16806000	-0.33297300	1.06012200
H	-3.33911900	1.52438400	-1.21167600
H	4.10609000	-0.17564900	-0.71298300

(MA)<sub>2</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>2</sub>

S	-2.11272000	0.07281000	-0.48724900
O	-1.43765200	-0.10670800	0.83847400
O	-1.14098200	-0.68268300	-1.49822100
O	-3.33760300	-0.64884900	-0.57409200
O	-2.10394800	1.46860300	-0.84722700
H	-0.88898900	-1.66992100	0.80616100
N	-0.05380200	2.22501600	0.84236300
H	-0.52187000	1.30063900	1.01086700
H	0.92628500	2.13230400	1.13329700
O	1.99307600	-1.31298700	0.12834200
O	2.45827000	0.95896700	0.89545100
S	2.20196600	0.07463300	-0.22051100
O	1.17857400	0.61132500	-1.11255100

O	3.54541200	0.01110500	-1.06507300
H	3.85392700	0.90813400	-1.23792800
H	-0.27063700	-0.21928200	-1.50872500
H	0.54110300	-2.17688500	0.18297400
N	-0.39119300	-2.53915200	0.47758600
C	-0.26846700	-3.57597400	1.51994900
C	-0.81790100	3.32091900	1.46861900
H	-1.82345600	3.29183200	1.06080400
H	-0.34737400	4.27285800	1.24502500
H	-0.84531000	3.16623100	2.54210300
H	-1.25686200	-3.86691700	1.86010100
H	0.25566100	-4.43745400	1.11912300
H	0.29853200	-3.16112200	2.34692900
H	-0.89406800	-2.85111600	-0.35085700
H	-0.06289900	2.29070400	-0.17758100

(MA)<sub>2</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>3</sub>

N	0.05440400	-2.03780700	-0.13473700
H	-0.81833400	-2.30447700	-0.61143900
H	0.87421100	-2.12201200	-0.74061100
N	-2.19003900	1.95735800	1.31859900
H	-3.16652000	2.23637900	1.26393900
H	-2.16942500	0.91857200	1.33262900
S	-3.03125700	-0.90144700	-0.24308300
O	-2.63143700	-2.09130000	-0.95949200
O	-2.86152400	0.34658800	-0.96452800
O	-2.44974200	-0.83151300	1.09375500
H	-1.31111600	0.47628300	-1.73168700
S	0.31644100	1.48851300	-0.84936400
O	-0.33498900	0.50960200	-1.88698600
O	1.63494000	1.75151700	-1.35374800
O	-0.55417700	2.63826400	-0.73343700
O	0.33795600	0.73542400	0.43027800
H	-0.01292300	-1.02851100	0.07483000
H	-1.71212200	2.25145300	0.43503200
O	-4.60495000	-0.98851500	-0.06027200
H	-4.85111900	-1.89538000	0.15871200
S	3.53944200	-0.55683500	0.19979200
O	3.94418300	0.66041400	-0.66154900
O	2.70415600	0.06383200	1.36015600
O	4.71004200	-1.10679000	0.76033700
O	2.65889900	-1.39151700	-0.56966300
H	3.13485600	1.09374900	-1.03886600
H	1.81257800	0.36525100	1.03075100

C	0.25123600	-2.78501200	1.12858800
H	0.32534000	-3.84515000	0.91143700
H	-0.60105700	-2.58578900	1.76981400
H	1.17051900	-2.43562600	1.58889300
C	-1.48661000	2.54295100	2.48144800
H	-1.53191500	3.62510600	2.41915400
H	-0.45340100	2.21577800	2.43320300
H	-1.94876200	2.19815500	3.40064700

(MA)<sub>3</sub>(H<sub>2</sub>SO<sub>4</sub>)

S	-0.60611700	-0.47495300	-0.57812900
O	-0.76625000	1.03404500	-0.12096500
O	-1.80465400	-0.82228100	-1.29094500
O	-0.45537400	-1.24255800	0.67661500
O	0.62918000	-0.48541700	-1.33173800
H	-1.75615100	1.22220200	0.02656000
H	2.29814900	-0.12001100	0.74090500
C	2.76411800	-2.10703900	0.23005100
H	3.83953300	-1.95282700	0.22961900
H	2.35985100	-1.97590700	-0.76857700
H	2.53417500	-3.10576600	0.58887800
N	2.10698000	-1.10588300	1.09589400
H	1.03251600	-1.21432100	1.02719400
N	-3.39420600	1.12003600	0.13973700
C	-3.67373700	0.20459200	1.25251600
H	-3.51152000	0.62978300	-0.74175700
H	-3.49575200	0.71966800	2.19424800
H	-4.69503800	-0.17925900	1.25020500
H	-2.98318100	-0.63391700	1.18676500
N	2.30056100	1.43947000	-0.05010700
C	3.20573800	2.57071500	0.14998100
H	2.29649200	1.12642700	-1.01582600
H	3.17208500	2.88368500	1.19185400
H	4.22700400	2.26630500	-0.07115400
H	2.96558100	3.43515700	-0.47212200
H	-4.01461000	1.91875500	0.14974400
H	1.33249200	1.70806500	0.11275200
H	2.40297100	-1.18406700	2.06308600

(MA)<sub>3</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>2</sub>

S	0.84453500	-1.74941600	-0.08299400
O	0.20412300	-1.00735500	1.01106500
N	1.44070900	1.48266500	0.89992600
H	0.86162300	0.66443000	1.16243000
O	2.13179800	-2.29465700	0.23431500

O	1.16639800	-0.65471900	-1.18486600
N	3.83616600	0.21486100	0.19445500
H	2.39442500	1.08828200	0.63232200
N	-2.33339000	-1.92644600	0.60492300
H	-2.45705800	-0.96441600	0.20614300
S	-1.72279500	1.57353200	-0.37179600
O	-0.55109200	1.40162000	-1.22996200
O	-1.39876200	1.91410500	0.98275900
O	-2.67984900	0.48936700	-0.53351000
H	0.40658700	-0.03908100	-1.30409100
O	-0.09881700	-2.69009600	-0.67228700
H	3.46110100	-0.73395900	0.21350400
H	4.63635900	0.22735700	0.81510700
H	0.97127100	1.85620600	0.07064500
H	-1.93393100	-1.80064300	1.53293100
H	-1.56310600	-2.36892700	0.04105600
O	-2.46209200	2.87004200	-0.92514900
H	-2.75645100	2.70091600	-1.82795000
C	4.24482900	0.55826300	-1.17274500
C	1.51745300	2.47703900	1.98571400
C	-3.59316600	-2.68991100	0.59746900
H	-4.34095200	-2.16551000	1.18386300
H	-3.42552500	-3.67984700	1.00982500
H	-3.93756100	-2.77728700	-0.42777300
H	0.51194600	2.80468200	2.22748400
H	1.98083200	2.01458200	2.85189300
H	2.11973200	3.32059100	1.66193800
H	3.36895200	0.51881600	-1.81590400
H	4.99662900	-0.11907200	-1.58040800
H	4.64455500	1.57068000	-1.19306400
(MA) <sub>3</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>3</sub>			
S	2.56371400	-1.20328200	0.02749300
O	2.64008700	-0.58816900	-1.27738400
O	3.90219400	-2.06144600	0.11385500
O	2.66500700	-0.22880900	1.10648200
H	3.87565500	-2.62061100	0.89993900
S	-2.92934100	-0.77171100	-0.16872700
O	-1.76867400	-1.50146600	0.38916100
O	-3.43451500	0.15456600	1.01882200
O	-2.50876300	0.13492000	-1.24760200
H	-2.79074000	0.88161800	1.19104900
S	-0.59956400	2.17392400	0.20799900
O	0.22893400	3.37067800	0.33720700

O	-1.40945600	1.92633300	1.40270500
O	0.15909600	0.95731100	-0.18263300
O	-1.56435600	2.49436700	-0.96093900
H	-2.08992800	1.67816100	-1.13380200
O	1.45867200	-2.11888500	0.21710300
N	2.68013900	2.34656500	-0.06318400
N	-0.06003000	-1.35097800	-1.69826000
N	-0.05881100	-0.59642800	2.16342000
H	-0.56095000	-0.44914700	-1.59402200
H	-0.14468300	-1.74714300	-0.75667700
H	0.92995200	-1.13836400	-1.89250600
H	-0.75293700	-0.96383200	1.44315200
H	-0.52725300	0.23433900	2.53332900
H	0.81732300	-0.31837200	1.72620100
H	1.79102100	2.84628000	0.19182000
H	2.61754600	1.37695400	0.27073100
H	3.47065100	2.78966100	0.39612700
O	-4.01179100	-1.61334400	-0.53309000
C	-0.72565000	-2.31488400	-2.65375600
C	2.79634700	2.36722200	-1.53122800
C	0.18663100	-1.66096100	3.15901200
H	-1.76430300	-2.48561000	-2.34069600
H	-0.18784500	-3.26068500	-2.63530100
H	-0.71046200	-1.88680100	-3.65621600
H	1.89583100	1.90828600	-1.92326400
H	3.66161200	1.78787100	-1.83126500
H	2.87354100	3.39810900	-1.86200700
H	-0.77373500	-1.99168700	3.55175700
H	0.80802800	-1.28333700	3.96604900
H	0.68022100	-2.48941900	2.65987600

(DMA)<sub>2</sub>

N	1.55417900	-0.00019600	-0.09426000
H	0.83934000	-0.00043300	0.62399800
H	-0.83939800	-0.00045200	-0.62411600
N	-1.55416900	-0.00019900	0.09420800
C	-2.35843100	1.20410100	-0.00791400
C	-2.35928600	-1.20393100	-0.00787200
C	2.35846000	1.20408500	0.00793400
C	2.35925600	-1.20394700	0.00789200
H	1.71664300	-2.08248900	-0.00436200
H	2.97799700	-1.23692400	0.91511700
H	3.02798500	-1.26413800	-0.85170200

H	3.02717300	1.26473500	-0.85164100
H	2.97715600	1.23744800	0.91517700
H	1.71526800	2.08220300	-0.00431700
H	-3.02794400	-1.26410000	0.85177800
H	-2.97810200	-1.23689600	-0.91504600
H	-1.71669300	-2.08248900	0.00433400
H	-2.97719700	1.23748400	-0.91510800
H	-3.02707500	1.26475800	0.85171300
H	-1.71521900	2.08220500	0.00429300

(DMA)<sub>3</sub>

N	0.57141300	1.71723900	-0.00419400
H	-0.34443500	1.27134100	0.00515600
H	1.26787600	-0.33891800	-0.02366500
N	1.20049700	-1.35531300	-0.01279100
C	1.81071000	-1.90465400	-1.20961200
C	1.80626800	-1.87532700	1.19936200
C	0.71372600	2.52822800	-1.19945100
C	0.75453900	2.49252500	1.20909400
H	0.56887000	1.86500500	2.07975000
H	0.09376900	3.36836900	1.26670000
H	1.78404400	2.84984500	1.26483000
H	1.74001500	2.89068400	-1.27718100
H	0.04929700	3.40311900	-1.21018400
H	0.50228800	1.92592000	-2.08190700
H	1.60861800	-2.94558700	1.27851200
H	2.89516200	-1.73341200	1.23427800
H	1.36849100	-1.38744400	2.06920200
H	2.89935500	-1.76100800	-1.24519800
H	1.61617900	-2.97714000	-1.26131600
H	1.37413200	-1.44118600	-2.09321500
N	-1.77433000	-0.36292000	0.00573900
H	-0.92854900	-0.93046900	-0.00318100
C	-2.54461300	-0.60541300	-1.20007200
C	-2.53873400	-0.63475500	1.20906800
H	-1.91377500	-0.46192700	-2.07630100
H	-2.97269200	-1.61633300	-1.24392900
H	-3.36957700	0.10643300	-1.25883000
H	-3.36274600	0.07603500	1.28975800
H	-2.96748200	-1.64613800	1.22978400
H	-1.90327400	-0.51386600	2.08532200

(DMA)(H<sub>2</sub>SO<sub>4</sub>)

H	1.50177100	-0.28871300	1.08036000
S	-1.26728500	-0.17446800	0.04950300

O	-1.68973800	1.32512100	-0.34652900
O	-0.33414200	-0.58684600	-1.02020500
O	-2.47301800	-0.93589500	0.07805600
O	-0.55359700	0.01427600	1.29369700
H	-2.46930300	1.27350500	-0.91061400
N	1.89016600	-0.11206500	0.15014300
H	1.04004800	-0.40415300	-0.47173600
C	3.10067500	-0.90093100	-0.11984000
H	3.90204600	-0.59322600	0.54772700
H	3.40249000	-0.73440600	-1.15034200
H	2.87989900	-1.95369300	0.02683100
C	2.05459400	1.34587300	-0.01688500
H	2.81894500	1.71345300	0.66340600
H	1.09786600	1.81497500	0.19664000
H	2.34397500	1.54530800	-1.04513000

(DMA)(H<sub>2</sub>SO<sub>4</sub>)<sub>2</sub>

S	1.41894300	-1.24254400	-0.10523600
O	2.26665900	-0.34101700	-0.84585700
O	0.87917800	-0.61387600	1.10411000
O	2.41316000	-2.37351300	0.37375900
O	0.39019200	-1.91454500	-0.87271200
H	1.76784800	1.27379700	-0.41944600
H	1.90968100	-3.14257900	0.66842400
S	-2.23151600	0.02605600	0.02736100
O	-1.69541200	-0.56516400	1.35193800
O	-3.59439100	0.34427200	0.18837800
O	-2.12517400	-1.13963300	-0.98073400
O	-1.32058200	1.06811300	-0.38960200
H	-0.69222000	-0.63037200	1.32633300
H	-1.18361500	-1.45972200	-1.04293800
N	1.17770100	2.05440100	-0.06994200
H	0.23850100	1.62082500	0.02260900
C	1.08211400	3.12715100	-1.08029600
H	2.06658300	3.55721300	-1.24201200
H	0.39576000	3.88805400	-0.71967900
H	0.70073300	2.69912900	-2.00196300
C	1.66754200	2.49855500	1.25080900
H	2.65684900	2.93247500	1.13455400
H	1.70857900	1.63202700	1.90279600
H	0.98159300	3.24082500	1.64958000

(DMA)(H<sub>2</sub>SO<sub>4</sub>)<sub>3</sub>

S	-1.11009200	1.71626000	-0.82091100
O	-1.88867900	1.48919200	0.39232600



O	0.30619400	1.85669900	-0.53089100
O	-1.62587600	3.12945100	-1.29092900
O	-1.39515800	0.79137000	-1.89413800
H	-0.58014800	0.95767700	1.69015300
H	-1.27632700	3.33338000	-2.16814500
S	-1.73406000	-1.84366100	0.03135400
O	-2.82324100	-0.94235500	0.65918300
O	-0.45600800	-1.22009800	0.32555200
O	-1.96340700	-1.74606200	-1.48963500
O	-1.96013800	-3.17047000	0.44002100
H	-2.59155700	0.02163700	0.54396600
H	-1.74577900	-0.82482400	-1.79721000
N	0.30586200	0.81084000	2.18819400
H	0.96225900	0.42539400	1.48327200
C	0.14425300	-0.17756600	3.27595800
H	-0.53920100	0.22007000	4.02096500
H	1.11885500	-0.35861000	3.72038200
H	-0.24655000	-1.09655700	2.85189100
C	0.84179000	2.11528800	2.63501600
H	0.17289400	2.53969300	3.37840100
H	0.91259900	2.76492700	1.76889400
H	1.82724100	1.95249900	3.06190900
S	2.79544500	-0.53626000	-0.53188000
O	4.12694300	-0.88325600	-0.82811900
O	2.33239400	0.52668000	-1.55611000
O	2.45893400	-0.05908100	0.78773700
H	1.54344800	1.03141700	-1.22548400
O	1.90717600	-1.77072100	-0.83180200
H	1.01119600	-1.66113700	-0.43474900

(DMA)<sub>2</sub>(H<sub>2</sub>SO<sub>4</sub>)

S	-0.04868500	0.82524000	0.01756500
O	0.65734700	-0.06769100	-1.06049700
O	0.96331600	1.63673200	0.63526000
O	-0.65152300	-0.13603500	0.98433800
O	-1.09915900	1.51905900	-0.69946500
H	1.62950200	-0.22554400	-0.76294400
H	-2.97432300	0.66863400	-0.33998700
C	-4.15870000	-0.61793400	0.80456500
H	-5.05532600	-0.58684800	0.18909700
H	-4.24263700	0.09976200	1.61501900
H	-4.03940500	-1.61587900	1.21836100
N	-2.97649700	-0.29740800	-0.00365600
C	-2.75573200	-1.19348900	-1.15522000

H	-2.02517600	-0.30057200	0.57257700
H	-3.60915100	-1.15594800	-1.82852500
H	-1.85218200	-0.86634600	-1.66372700
H	-2.62134200	-2.20562600	-0.78256300
N	3.05033800	-0.27816500	-0.01436100
C	4.27684600	-0.64209000	-0.70867700
C	2.81163800	-1.07909400	1.18406300
H	3.05390200	0.70355700	0.24609000
H	4.18821300	-1.66259600	-1.08015000
H	4.42925700	0.01922800	-1.55854400
H	5.15633900	-0.59200900	-0.05832500
H	2.66928400	-2.11951800	0.89202500
H	3.64656800	-1.02892400	1.88989100
H	1.90440200	-0.72707100	1.67131200

(DMA)<sub>2</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>2</sub>

H	-0.53850600	-1.41133100	0.27351400
S	2.55661000	-0.08252700	-0.25327900
O	3.94685400	-0.09478000	0.53205900
O	2.42397800	-1.40178200	-0.85179100
O	2.61665000	0.99994000	-1.19767700
O	1.59293600	0.12728800	0.82079500
H	4.66198400	-0.14808000	-0.11291300
N	0.02982000	-2.27544800	0.17346100
H	0.91799800	-2.00185600	-0.29704100
C	-0.70114200	-3.27228500	-0.63441200
H	-1.66293400	-3.46417600	-0.16795700
H	-0.10986500	-4.18306500	-0.68401400
H	-0.86902400	-2.86417900	-1.62464300
C	0.34962200	-2.73095100	1.54201600
H	-0.57891600	-2.95300500	2.06097200
H	0.88076300	-1.92862800	2.04392500
H	0.97175400	-3.62010800	1.48500600
H	0.53847800	1.41144300	0.27320700
S	-2.55657700	0.08243700	-0.25338900
O	-3.94684800	0.09499000	0.53189500
O	-1.59294900	-0.12705300	0.82079100
O	-2.42387500	1.40148800	-0.85233000
O	-2.61659800	-1.00034200	-1.19742700
H	-4.66195200	0.14814200	-0.11311500
N	-0.02985900	2.27552700	0.17294000
H	-0.91799600	2.00180100	-0.29756700
C	0.70112400	3.27219100	-0.63513100
H	1.66286700	3.46425000	-0.16864000

H	0.10981100	4.18293200	-0.68500800
H	0.86911400	2.86383000	-1.62523800
C	-0.34975900	2.73134300	1.54136400
H	0.57873800	2.95354800	2.06032900
H	-0.88091400	1.92912800	2.04342900
H	-0.97191200	3.62047000	1.48409900

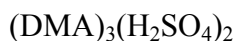
(DMA)<sub>2</sub>(H<sub>2</sub>SO<sub>4</sub>)<sub>3</sub>

S	1.29721500	-1.97900500	-0.55955600
O	2.67764800	-1.95599500	-0.91182000
O	0.84225600	-3.47269600	-0.60904800
O	1.04594200	-1.51434000	0.81427400
O	0.43459300	-1.25848100	-1.51306600
H	-1.78347400	1.11048800	0.00585700
N	3.07985500	0.57365800	0.95430800
H	2.36729700	-0.17117500	0.91068700
H	2.81688000	1.25162900	0.20181600
O	0.33515200	1.30286700	0.43486800
O	2.08615900	2.43752100	-0.77004200
S	0.65476500	2.21851200	-0.65722100
O	-0.15338700	3.41580500	-0.65170800
O	0.17988700	1.47507400	-1.97579400
H	0.49444300	0.55016900	-1.95835800
H	-0.08925400	-3.53082800	-0.31685000
H	-1.77424700	2.71821100	-0.13901400
N	-2.39002900	1.92909300	0.13274000
C	-2.73685900	2.01734500	1.56846200
C	-3.55443800	1.82161700	-0.77205800
C	4.42711900	0.01436800	0.71520700
C	2.94172700	1.27234800	2.24994400
H	1.92297100	1.63839200	2.32393300
H	3.64255100	2.10199700	2.27619300
H	3.15834600	0.57451300	3.05423300
H	4.64739000	-0.71456400	1.49042100
H	5.14973000	0.82509300	0.74840900
H	4.43269800	-0.47330900	-0.25288200
H	-4.11709500	0.93226800	-0.50182700
H	-4.16619400	2.71271600	-0.66322100
H	-3.18810800	1.73422900	-1.79001000
H	-3.31209500	2.92353300	1.73553800
H	-3.31567900	1.13720800	1.83513700
H	-1.81025400	2.03803200	2.13297600
S	-2.25192800	-1.54901600	0.42307000
O	-3.59977900	-1.28619000	0.77363300

O	-1.97205400	-0.77795700	-0.89832200
O	-1.78089500	-2.89163000	0.27247000
H	-1.02322900	-0.98724400	-1.21760200
O	-1.36527800	-0.81024000	1.45655800
H	-0.38950900	-1.00243100	1.26920600

(DMA)<sub>3</sub>(H<sub>2</sub>SO<sub>4</sub>)

S	-0.64261900	-0.25121900	-0.66966800
O	-1.94048000	-0.52887600	-1.48036700
O	0.42703900	-0.14209600	-1.63959200
O	-0.44063100	-1.41392800	0.21753800
O	-0.85906900	0.96421600	0.10135400
H	-2.75224300	-0.41797600	-0.86160300
H	2.23583700	-0.19201300	0.30898600
C	2.86652200	-1.86355300	-0.78489800
H	3.91105700	-1.55772600	-0.80203000
H	2.34965600	-1.51578200	-1.67422700
H	2.80627300	-2.94768700	-0.71748800
N	2.19961100	-1.26321400	0.38216900
C	2.75742200	-1.67773100	1.67540500
H	1.15757300	-1.46860400	0.34479100
H	3.80580800	-1.39093200	1.73098900
H	2.20223900	-1.18797200	2.47076700
H	2.67079200	-2.75632900	1.78499300
N	-3.92360400	-0.13836200	0.20845500
C	-4.14018100	1.30833100	0.21751800
C	-3.44144300	-0.63079600	1.50052500
H	-4.78261900	-0.61423000	-0.03891300
H	-3.17459600	1.79074500	0.35807700
H	-4.54769500	1.62266200	-0.74095000
H	-4.82035600	1.61994700	1.01656200
H	-2.48988400	-0.14762800	1.71395700
H	-4.14574100	-0.41613100	2.31055300
H	-3.26733200	-1.70254300	1.44092500
N	2.15283000	1.51450100	0.21750500
C	2.80274000	1.93340200	-1.02024800
C	2.57173500	2.30688400	1.36546700
H	1.14173100	1.58472600	0.10223200
H	3.87391500	1.73354300	-0.95591500
H	2.37689400	1.36919700	-1.84671700
H	2.67095800	3.00289300	-1.21578000
H	3.63048200	2.13426400	1.56490000
H	2.43072600	3.38133400	1.20566100
H	2.00094400	2.01154600	2.24393100



S	1.26195200	-0.43743200	-0.90393500
O	2.64725700	-0.17992900	-1.37754100
C	-2.27783300	-3.06774500	0.22410100
H	-3.34480500	-3.04083600	0.01735000
H	-1.90202900	-4.08149500	0.10919800
H	-2.09461900	-2.70373600	1.23079500
N	3.76739900	0.03352700	0.89156400
H	3.43211300	-0.02570300	-0.16654900
H	2.97507500	0.53476900	1.30090000
C	5.03472100	0.75492400	1.06353400
C	3.77412400	-1.34774100	1.41657800
H	4.54033400	-1.91025800	0.88953800
H	2.80039700	-1.78926600	1.21793600
H	3.98627400	-1.33870300	2.48319300
H	5.81643200	0.21833600	0.53251000
H	4.93795000	1.75341300	0.64780000
H	5.29096100	0.81663000	2.11901300
O	1.09545300	-1.86407400	-0.58470600
O	0.27692000	-0.01104300	-1.90460300
N	-1.58425600	-2.17682300	-0.72325900
C	-1.79155200	-2.51284400	-2.14215200
H	-1.91902500	-1.19557400	-0.53327000
H	-0.55182700	-2.15669500	-0.54337200
H	-1.46341300	-3.53418200	-2.32004100
H	-1.19979900	-1.82359800	-2.73729300
H	-2.84788300	-2.41804100	-2.38190400
C	0.40329000	3.18195000	-1.08519200
H	1.23030100	2.69325100	-0.58002900
H	0.20260000	4.15260000	-0.63840500
H	0.63433200	3.29836500	-2.14117500
N	-0.78410400	2.32392500	-0.94247500
C	-1.98466600	2.84005400	-1.62353900
H	-1.01986000	2.17961600	0.07329100
H	-0.53813700	1.37803300	-1.30892700
H	-2.79810000	2.14757700	-1.43347800
H	-2.22750400	3.81946600	-1.21877500
H	-1.78660700	2.91935500	-2.68974000
S	-2.18165200	0.46658800	1.42069900
O	-3.20677900	0.09040100	2.33687800
O	-0.96989400	-0.50608000	1.72740200
O	-1.65724100	1.82382300	1.55846400
O	-2.51307000	0.21344100	0.00286200

O	1.07423400	0.36585300	0.34770900
H	-0.15477800	-0.17494200	1.25070800
(DMA) <sub>3</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>3</sub>			
S	-0.60487200	-1.89418900	-0.73520900
O	0.57139800	-2.73632100	-0.72691500
O	-1.75826700	-2.53162800	-1.34512700
O	-0.93830900	-1.32226400	0.56648300
O	-0.20944300	-0.67946600	-1.66081300
H	0.35558300	2.39719200	-0.27545600
N	2.67216700	-2.39970200	0.92189200
H	1.92811200	-2.34349300	0.19273700
H	3.34941500	-1.63106000	0.71988700
O	1.70480400	0.43978600	0.36681300
O	4.05694500	-0.15645000	0.20923800
S	2.91771800	0.46617000	-0.43815700
O	3.20346300	1.78181000	-0.98093500
O	2.62119300	-0.50014500	-1.66193000
H	1.65732600	-0.54791100	-1.81076300
H	-3.13081100	-1.84201500	-0.66506300
H	1.91166200	2.80267800	-0.55048600
N	1.01720100	3.17591200	-0.16501800
C	1.19686100	3.46056400	1.27653100
C	0.52190400	4.32764200	-0.94496400
C	3.31622500	-3.71982400	0.80517300
C	2.02126800	-2.15623900	2.22561100
H	1.59570900	-1.15795100	2.19989600
H	2.76233300	-2.24055700	3.01630000
H	1.23450300	-2.89350200	2.36275800
H	2.55866400	-4.48967500	0.92518800
H	4.07767200	-3.82043200	1.57399200
H	3.76778000	-3.80200900	-0.17862000
H	-0.44506800	4.61784800	-0.54460500
H	1.23780700	5.14077300	-0.86207000
H	0.41805600	4.02633400	-1.98272000
H	1.94483500	4.24218100	1.38119400
H	0.24103900	3.77423900	1.68503500
H	1.52736400	2.54437100	1.75419000
S	-1.94818400	1.81191100	0.46283000
O	-1.96058800	3.21185100	0.76004800
O	-1.30489700	1.51079900	-0.83111100
O	-3.23244900	1.14221200	0.58763300
H	-0.65836600	0.16201500	-1.33972500
O	-0.97967100	1.18897300	1.54111800

H	-0.76331800	0.26810500	1.26746900
N	-3.85945500	-1.33966600	-0.10975600
C	-4.03379700	-2.02676800	1.18459100
C	-5.10582900	-1.18820300	-0.88013800
H	-3.47853300	-0.38161500	0.09539900
H	-4.45647100	-3.01384800	1.01519900
H	-3.05703600	-2.10951400	1.65064700
H	-4.69829600	-1.43482200	1.80871400
H	-5.53196000	-2.16842700	-1.07779900
H	-5.80405200	-0.58722400	-0.30346700
H	-4.88116100	-0.68604600	-1.81593000