

Supporting Information

Gas-phase aldol condensation of formaldehyde to produce hydroxyacetaldehyde and its implication to new particle formation: a theoretical study

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Table S1. Cluster formation energies from monomers computed at the PW91/6-311++G(3df, 3pd) level of theory for $(\text{H}_2\text{SO}_4)_m(\text{C}_2\text{H}_4\text{O}_2)_n$ ($0 \leq m, n \leq 3$) clusters. All values are at 298.15 K and 1atm reference pressure in kcal mol⁻¹.

Cluster	ΔE_{elec}	ΔH	ΔS
$(\text{H}_2\text{SO}_4)_2$	-17.38	-16.54	-0.04
$(\text{H}_2\text{SO}_4)_3$	-33.26	-31.73	-0.08
$(\text{C}_2\text{H}_4\text{O}_2)_2$	-9.56	-7.48	-0.03
$(\text{C}_2\text{H}_4\text{O}_2)_3$	-21.32	-18.01	-0.07
$(\text{H}_2\text{SO}_4)(\text{C}_2\text{H}_4\text{O}_2)$	-12.48	-11.16	-0.03
$(\text{H}_2\text{SO}_4)_2(\text{C}_2\text{H}_4\text{O}_2)$	-32.10	-30.45	-0.07
$(\text{H}_2\text{SO}_4)_3(\text{C}_2\text{H}_4\text{O}_2)$	-49.42	-47.18	-0.12
$(\text{H}_2\text{SO}_4)(\text{C}_2\text{H}_4\text{O}_2)_2$	-27.02	-24.15	-0.07
$(\text{H}_2\text{SO}_4)_2(\text{C}_2\text{H}_4\text{O}_2)_2$	-47.18	-43.53	-0.11
$(\text{H}_2\text{SO}_4)_3(\text{C}_2\text{H}_4\text{O}_2)_2$	-67.71	-63.72	-0.15
$(\text{H}_2\text{SO}_4)(\text{C}_2\text{H}_4\text{O}_2)_3$	-43.23	-38.84	-0.11
$(\text{H}_2\text{SO}_4)_2(\text{C}_2\text{H}_4\text{O}_2)_3$	-60.67	-55.94	-0.15
$(\text{H}_2\text{SO}_4)_3(\text{C}_2\text{H}_4\text{O}_2)_3$	-74.17	-69.26	-0.19

Table S2. Coordinates of optimized global free energy minima obtained at the PW91PW91/6-311++G(3df, 3pd) level of theory for $(\text{H}_2\text{SO}_4)_m(\text{C}_2\text{H}_4\text{O}_2)_n$ ($0 \leq m, n \leq 3$), $(\text{SA})_m(\text{H}_2\text{O})$ ($0 \leq m \leq 3$), and $(\text{H}_2\text{SO}_4)_m(\text{NH}_3)$ ($0 \leq m \leq 3$).

$\text{C}_2\text{H}_4\text{O}_2$

C	-0.727944000000	-0.352813000000	0.099762000000
O	-1.848672000000	0.056456000000	-0.099420000000
H	-0.521784000000	-1.426009000000	0.346931000000
C	0.515705000000	0.520930000000	0.050344000000
H	0.423253000000	1.229156000000	-0.788723000000
H	0.531103000000	1.119694000000	0.973617000000
O	1.724458000000	-0.221634000000	0.027048000000
H	1.834577000000	-0.610117000000	-0.853489000000

$(\text{H}_2\text{SO}_4)_1(\text{C}_2\text{H}_4\text{O}_2)_1$

C	-2.006182000000	0.337673000000	-0.199256000000
O	-1.327346000000	1.324341000000	0.048637000000
H	-1.568059000000	-0.550438000000	-0.702013000000
C	-3.468956000000	0.251230000000	0.162644000000

H	-3.592933000000	0.579943000000	1.208704000000
H	-4.004140000000	0.986406000000	-0.458126000000
O	-4.041399000000	-1.012585000000	-0.103873000000
H	-3.732624000000	-1.649007000000	0.558552000000
S	1.795926000000	-0.218238000000	-0.099999000000
O	0.751635000000	-1.206135000000	-0.198108000000
O	3.066849000000	-0.365957000000	-0.751225000000
O	1.234423000000	1.198301000000	-0.502212000000
O	2.050612000000	-0.070509000000	1.492905000000
H	0.239173000000	1.251503000000	-0.289110000000
H	2.896414000000	0.400352000000	1.612662000000

(H₂SO₄)₂(C₂H₄O₂)₁

C	1.931953000000	-1.478253000000	-0.698415000000
O	1.066774000000	-2.051490000000	-0.041430000000
H	1.673329000000	-0.838853000000	-1.563267000000
C	3.372634000000	-1.615605000000	-0.355722000000
H	3.890847000000	-1.984352000000	-1.263061000000
H	3.753829000000	-0.589397000000	-0.189191000000
O	3.623605000000	-2.446668000000	0.740466000000
H	2.757187000000	-2.734274000000	1.084941000000
S	-2.308671000000	-0.874137000000	0.101654000000
O	-1.496751000000	-0.335473000000	1.207074000000
O	-3.618318000000	-1.365472000000	0.374607000000
O	-2.453942000000	0.246077000000	-1.001756000000
O	-1.472638000000	-2.003950000000	-0.589630000000
H	-1.587032000000	0.738237000000	-1.114156000000
H	-0.480216000000	-1.964361000000	-0.348490000000
S	0.662106000000	1.976550000000	-0.006288000000
O	-0.122526000000	1.541693000000	-1.162523000000
O	1.985737000000	1.444185000000	0.142467000000
O	0.847200000000	3.556993000000	-0.061751000000
O	-0.199057000000	1.834797000000	1.282860000000
H	-0.022243000000	3.982739000000	-0.190693000000
H	-0.748861000000	0.949245000000	1.259802000000

(H₂SO₄)₃(C₂H₄O₂)₁

C	5.053977000000	-0.501388000000	0.987333000000
O	4.183556000000	-1.327718000000	1.222202000000
H	5.819967000000	-0.292061000000	1.765999000000
C	5.199324000000	0.304540000000	-0.267943000000
H	5.152390000000	1.368331000000	0.056256000000
H	6.240839000000	0.166642000000	-0.608393000000
O	4.346342000000	-0.006199000000	-1.321038000000

H	3.420384000000	0.197415000000	-1.073525000000
S	-0.981215000000	2.678186000000	-0.033310000000
O	-1.433915000000	4.009400000000	-0.300491000000
O	-1.514953000000	1.528270000000	-0.742328000000
O	0.576926000000	2.667477000000	-0.167596000000
O	-1.244658000000	2.327020000000	1.514639000000
H	0.937670000000	1.720394000000	-0.239944000000
H	-1.218336000000	3.158138000000	2.025716000000
S	1.004810000000	-0.983629000000	-0.144092000000
O	0.148803000000	-0.991194000000	1.031030000000
O	1.682234000000	0.304157000000	-0.395621000000
O	2.098778000000	-2.073207000000	-0.069678000000
O	0.231238000000	-1.413970000000	-1.398950000000
H	2.962429000000	-1.730038000000	0.387892000000
H	-0.786230000000	-1.576526000000	-1.209739000000
S	-3.195331000000	-1.485586000000	-0.008273000000
O	-2.210008000000	-1.861141000000	-1.033600000000
O	-4.379894000000	-2.265312000000	0.119897000000
O	-2.462270000000	-1.458263000000	1.388303000000
O	-3.642357000000	0.000094000000	-0.256266000000
H	-1.482766000000	-1.286600000000	1.269583000000
H	-2.856947000000	0.596559000000	-0.443403000000

(C₂H₄O₂)₂

C	-1.669013000000	1.092523000000	-0.240568000000
O	-0.712044000000	1.812516000000	-0.016646000000
H	-2.319629000000	1.281001000000	-1.125499000000
C	-2.036005000000	-0.148594000000	0.545064000000
H	-1.346566000000	-0.284048000000	1.391306000000
H	-3.059458000000	-0.040014000000	0.935067000000
O	-2.030771000000	-1.245019000000	-0.357564000000
H	-1.097067000000	-1.529512000000	-0.452119000000
C	1.669031000000	-1.091828000000	0.242610000000
O	0.711502000000	-1.812470000000	0.023196000000
H	2.321867000000	-1.277767000000	1.126432000000
C	2.034340000000	0.147040000000	-0.547440000000
H	3.056536000000	0.036619000000	-0.940195000000
H	1.342531000000	0.280734000000	-1.392058000000
O	2.032841000000	1.246003000000	0.352040000000
H	1.099446000000	1.529905000000	0.450863000000

(H₂SO₄)₁(C₂H₄O₂)₂

C	0.301141000000	-2.473168000000	0.905206000000
O	-0.711111000000	-2.030229000000	1.433780000000

H	1.098713000000	-2.921376000000	1.537004000000
C	0.594474000000	-2.469802000000	-0.572892000000
H	0.107222000000	-3.370569000000	-0.988003000000
H	0.104491000000	-1.599325000000	-1.039169000000
O	1.972404000000	-2.557511000000	-0.838783000000
H	2.367469000000	-1.667097000000	-0.693997000000
C	2.700346000000	2.285268000000	0.178478000000
O	3.302277000000	2.055007000000	1.210159000000
H	2.309425000000	3.296881000000	-0.062073000000
C	2.451443000000	1.199565000000	-0.828080000000
H	1.362854000000	1.115954000000	-0.988649000000
H	2.900956000000	1.502589000000	-1.790816000000
O	3.001903000000	-0.022549000000	-0.376043000000
H	3.422427000000	0.193886000000	0.486101000000
S	-2.196986000000	0.681025000000	-0.266207000000
O	-3.297102000000	1.200448000000	-1.027407000000
O	-0.854130000000	0.638240000000	-0.794663000000
O	-2.045260000000	1.547155000000	1.093142000000
O	-2.622662000000	-0.736368000000	0.252082000000
H	-2.942027000000	1.781053000000	1.398161000000
H	-1.834737000000	-1.233121000000	0.686347000000

(H₂SO₄)₂(C₂H₄O₂)₂

C	-1.202755000000	3.025902000000	1.205374000000
O	-1.035512000000	3.956584000000	0.439087000000
H	-2.202309000000	2.734355000000	1.579541000000
C	-0.019344000000	2.221420000000	1.674760000000
H	0.050774000000	2.276906000000	2.773328000000
H	-0.167222000000	1.166461000000	1.402361000000
O	1.161422000000	2.746017000000	1.074392000000
H	0.834043000000	3.499196000000	0.521894000000
C	0.166719000000	-2.251580000000	2.016669000000
O	0.695116000000	-1.425199000000	2.738605000000
H	-0.894446000000	-2.545687000000	2.125151000000
C	0.960489000000	-2.910598000000	0.920470000000
H	0.972225000000	-4.001041000000	1.084656000000
H	0.458696000000	-2.722047000000	-0.040405000000
O	2.287016000000	-2.392455000000	0.919213000000
H	2.305961000000	-1.782234000000	1.696885000000
S	2.019325000000	0.261450000000	-1.231682000000
O	0.651496000000	-0.039368000000	-0.766133000000
O	2.170675000000	0.886875000000	-2.510596000000
O	2.716340000000	1.068503000000	-0.081349000000
O	2.855659000000	-1.054916000000	-1.222899000000

H	2.068528000000	1.754338000000	0.340780000000
H	2.661744000000	-1.589364000000	-0.365732000000
S	-2.554261000000	-0.691954000000	-0.492980000000
O	-2.619006000000	0.251595000000	0.592427000000
O	-2.136841000000	-2.052962000000	-0.227558000000
O	-4.014450000000	-0.701214000000	-1.145859000000
O	-1.747693000000	-0.106335000000	-1.709972000000
H	-4.072884000000	-1.453995000000	-1.764069000000
H	-0.760579000000	-0.056690000000	-1.458298000000

(H₂SO₄)₃(C₂H₄O₂)₂

C	2.477227000000	2.003583000000	-1.130214000000
O	3.411363000000	2.558530000000	-0.592198000000
H	3.301091000000	0.245168000000	-1.305330000000
C	1.125983000000	2.672941000000	-1.330316000000
H	0.851700000000	3.153346000000	-0.382289000000
H	1.229717000000	3.454307000000	-2.094124000000
O	0.085787000000	1.766648000000	-1.748168000000
H	0.416824000000	0.839313000000	-1.672287000000
C	6.365012000000	-1.212746000000	0.599333000000
O	7.082405000000	-1.159075000000	1.570222000000
H	6.624083000000	-1.820903000000	-0.303749000000
C	5.052324000000	-0.457332000000	0.488326000000
H	4.489195000000	-0.558391000000	1.426803000000
H	5.273647000000	0.612338000000	0.355548000000
O	4.289875000000	-0.879879000000	-0.650023000000
H	3.677975000000	-1.597543000000	-0.392897000000
S	-1.764532000000	1.962528000000	1.121371000000
O	-1.854609000000	3.360036000000	1.415879000000
O	-0.579915000000	1.206199000000	1.464297000000
O	-3.054372000000	1.275064000000	1.731009000000
O	-2.048469000000	1.732820000000	-0.451456000000
H	-2.977411000000	0.291186000000	1.613694000000
H	-1.119636000000	1.782103000000	-0.991736000000
S	-3.669900000000	-1.460466000000	-0.387841000000
O	-2.846371000000	-1.320708000000	0.815472000000
O	-3.721712000000	-2.704198000000	-1.090854000000
O	-5.127029000000	-1.068639000000	0.152087000000
O	-3.322773000000	-0.329776000000	-1.399257000000
H	-5.787372000000	-1.293206000000	-0.531524000000
H	-2.861225000000	0.475571000000	-0.960897000000
S	0.717266000000	-1.322803000000	0.270993000000
O	0.054443000000	-0.992971000000	-1.001270000000
O	2.479872000000	0.753648000000	-1.607590000000

O	-0.265567000000	-2.391400000000	1.024041000000
O	1.907444000000	-2.456353000000	-0.021339000000
H	-1.194421000000	-2.045823000000	0.959724000000
H	1.504231000000	-3.243842000000	-0.442895000000

(C₂H₄O₂)₃

C	1.912835000000	1.744008000000	-0.179531000000
O	2.634918000000	1.032356000000	0.498932000000
H	1.974149000000	1.737661000000	-1.293625000000
C	0.832931000000	2.648112000000	0.369909000000
H	0.586099000000	2.331958000000	1.396843000000
H	1.250722000000	3.667451000000	0.430665000000
O	-0.277272000000	2.687419000000	-0.496909000000
H	-0.748346000000	1.819717000000	-0.436686000000
C	1.228643000000	-1.712893000000	-0.290946000000
O	0.213573000000	-1.664203000000	0.385823000000
H	1.236215000000	-1.350174000000	-1.345755000000
C	2.572803000000	-2.188177000000	0.203255000000
H	2.585026000000	-2.160354000000	1.304749000000
H	2.693803000000	-3.239599000000	-0.106052000000
O	3.614387000000	-1.446743000000	-0.394384000000
H	3.502113000000	-0.512710000000	-0.109284000000
C	-3.814066000000	-0.729546000000	-0.318066000000
O	-4.885620000000	-1.031773000000	0.153390000000
H	-3.481035000000	-1.090606000000	-1.324359000000
C	-2.810005000000	0.172277000000	0.384047000000
H	-3.246302000000	1.181158000000	0.432306000000
H	-2.687643000000	-0.176786000000	1.421620000000
O	-1.574051000000	0.261752000000	-0.309304000000
H	-1.011142000000	-0.520867000000	-0.082810000000

(H₂SO₄)₁(C₂H₄O₂)₃

C	1.990232000000	2.806697000000	-0.290335000000
O	1.028550000000	2.774954000000	-1.045188000000
H	2.849408000000	3.476192000000	-0.517879000000
C	2.147480000000	2.004767000000	0.977601000000
H	1.602125000000	2.560945000000	1.763155000000
H	1.636609000000	1.035122000000	0.869607000000
O	3.499389000000	1.894683000000	1.353394000000
H	3.853386000000	1.050842000000	0.986565000000
C	3.166352000000	-2.502103000000	-0.276425000000
O	3.234372000000	-2.886055000000	0.875263000000
H	2.635050000000	-3.077669000000	-1.061989000000
C	3.821481000000	-1.212547000000	-0.692752000000

H	4.592715000000	-1.443340000000	-1.450308000000
H	3.061823000000	-0.579898000000	-1.175977000000
O	4.392824000000	-0.568682000000	0.431222000000
H	4.262112000000	-1.207823000000	1.169060000000
C	-5.491049000000	-0.404216000000	0.060743000000
O	-5.664391000000	0.789607000000	0.213166000000
H	-6.190933000000	-1.031023000000	-0.531089000000
C	-4.303397000000	-1.090237000000	0.672253000000
H	-4.652580000000	-1.895607000000	1.340098000000
H	-3.700633000000	-1.551587000000	-0.129028000000
O	-3.527977000000	-0.145159000000	1.396937000000
H	-3.995871000000	0.712599000000	1.262117000000
S	-0.718420000000	-0.322910000000	-0.691921000000
O	0.683913000000	-0.645909000000	-0.833155000000
O	-1.731874000000	-1.180018000000	-1.257078000000
O	-0.957953000000	-0.165012000000	0.866152000000
O	-0.993316000000	1.119266000000	-1.265757000000
H	-1.955345000000	-0.129206000000	1.059637000000
H	-0.198020000000	1.731460000000	-1.099390000000

(H₂SO₄)₂(C₂H₄O₂)₃

C	-2.596048000000	2.695215000000	-0.918007000000
O	-3.788897000000	2.496718000000	-0.824842000000
H	-2.079240000000	2.741476000000	-1.905329000000
C	-1.690604000000	2.915567000000	0.281303000000
H	-1.790066000000	3.971669000000	0.576602000000
H	-2.046502000000	2.303479000000	1.123784000000
O	-0.320580000000	2.684248000000	-0.021998000000
H	-0.172422000000	1.714805000000	-0.033457000000
C	-5.891402000000	-1.119241000000	0.413749000000
O	-6.016171000000	-1.726602000000	1.460735000000
H	-6.753146000000	-0.908150000000	-0.252511000000
C	-4.544956000000	-0.616627000000	-0.018211000000
H	-4.281423000000	-1.047075000000	-0.998210000000
H	-4.577506000000	0.477860000000	-0.150200000000
O	-3.579296000000	-0.970607000000	0.969225000000
H	-4.095124000000	-1.467312000000	1.650180000000
C	3.229858000000	2.183291000000	0.311190000000
O	3.650900000000	1.584080000000	-0.671594000000
H	3.032233000000	1.649136000000	1.265246000000
C	2.895935000000	3.651795000000	0.314575000000
H	3.787766000000	4.187684000000	0.683013000000
H	2.720224000000	3.985667000000	-0.721383000000
O	1.831065000000	3.931952000000	1.192016000000

H	1.012999000000	3.535302000000	0.807631000000
S	3.316876000000	-1.790185000000	0.350988000000
O	4.350231000000	-2.380799000000	1.139897000000
O	2.343134000000	-0.928564000000	1.056893000000
O	3.894995000000	-0.969358000000	-0.849004000000
O	2.554812000000	-2.949258000000	-0.378074000000
H	3.808390000000	0.046902000000	-0.701778000000
H	1.734491000000	-2.592717000000	-0.839782000000
S	-0.630569000000	-1.093751000000	-0.789651000000
O	0.366667000000	-1.897855000000	-1.474209000000
O	-1.542628000000	-0.281289000000	-1.552296000000
O	-1.409676000000	-2.067778000000	0.149795000000
O	0.111386000000	-0.099588000000	0.200329000000
H	-2.280355000000	-1.628457000000	0.490903000000
H	1.014512000000	-0.489685000000	0.541340000000

(H₂SO₄)₃(C₂H₄O₂)₃

C	-3.033983000000	2.829649000000	-1.400397000000
O	-4.038262000000	2.441254000000	-0.826501000000
H	-2.424881000000	2.151700000000	-2.033598000000
C	-2.568955000000	4.249668000000	-1.294126000000
H	-1.526542000000	4.225534000000	-0.925987000000
H	-2.521212000000	4.662447000000	-2.320962000000
O	-3.387043000000	5.031332000000	-0.468404000000
H	-4.095128000000	4.433486000000	-0.156465000000
C	-5.020818000000	-0.406993000000	0.198713000000
O	-4.956475000000	-1.604492000000	0.492060000000
H	-4.230563000000	0.094631000000	-0.384409000000
C	-6.174259000000	0.416848000000	0.633337000000
H	-5.756356000000	1.272322000000	1.200203000000
H	-6.603662000000	0.874710000000	-0.279740000000
O	-7.141229000000	-0.273020000000	1.369952000000
H	-6.836217000000	-1.195477000000	1.455405000000
C	1.027028000000	1.337095000000	1.902472000000
O	2.182582000000	1.347876000000	2.296866000000
H	0.223024000000	0.930979000000	2.554698000000
C	0.559557000000	1.874317000000	0.569830000000
H	0.714941000000	2.965928000000	0.600806000000
H	1.222074000000	1.492357000000	-0.222412000000
O	-0.810842000000	1.643639000000	0.328230000000
H	-0.953430000000	0.725479000000	0.022018000000
S	2.258373000000	-1.933628000000	-0.249480000000
O	3.592982000000	-2.137007000000	0.276799000000
O	1.266768000000	-1.408899000000	0.694114000000

O	2.305765000000	-1.014140000000	-1.508649000000
O	1.759379000000	-3.273707000000	-0.845905000000
H	2.898223000000	-0.194018000000	-1.306881000000
H	0.754869000000	-3.221479000000	-1.037292000000
S	4.884166000000	1.253231000000	-0.076351000000
O	3.659450000000	1.038171000000	-0.869604000000
O	5.974811000000	1.962270000000	-0.658734000000
O	4.471788000000	2.003109000000	1.231544000000
O	5.420564000000	-0.151003000000	0.400231000000
H	3.549587000000	1.732386000000	1.571834000000
H	4.712165000000	-0.858883000000	0.394917000000
S	-1.655064000000	-2.278891000000	-0.352804000000
O	-1.849706000000	-0.869950000000	-0.652830000000
O	-0.798688000000	-3.037490000000	-1.257667000000
O	-1.113989000000	-2.437555000000	1.123718000000
O	-3.000935000000	-3.018246000000	-0.263544000000
H	-0.167993000000	-2.088189000000	1.120400000000
H	-3.785266000000	-2.395957000000	0.053251000000

H₂O

O	0.000000000000	0.118882000000	0.000000000000
H	0.764475000000	-0.475529000000	0.000000000000
H	-0.764475000000	-0.475529000000	0.000000000000

(H₂SO₄)(H₂O)

S	0.574100000000	0.074192000000	0.128480000000
O	-0.228971000000	-0.386595000000	1.239489000000
O	1.737470000000	0.893765000000	0.309622000000
O	1.015548000000	-1.280946000000	-0.628258000000
O	-0.358121000000	0.786822000000	-0.923700000000
H	1.765860000000	-1.065191000000	-1.213280000000
H	-1.320419000000	0.493113000000	-0.746103000000
O	-2.677872000000	-0.107847000000	-0.117951000000
H	-3.322309000000	0.552297000000	0.179793000000
H	-2.213170000000	-0.408888000000	0.690302000000

(H₂SO₄)₂(H₂O)

S	1.820061000000	-0.360864000000	-0.014994000000
O	2.380761000000	1.060200000000	-0.131115000000
O	1.120750000000	-0.532274000000	1.255078000000
O	3.150529000000	-1.233817000000	0.000554000000
O	1.122822000000	-0.777854000000	-1.216230000000
H	1.573735000000	1.831996000000	-0.042718000000
H	3.627045000000	-1.077866000000	0.838605000000

S	-2.136651000000	-0.117731000000	-0.005287000000
O	-1.579644000000	-0.747590000000	1.333364000000
O	-3.555119000000	-0.249001000000	0.016653000000
O	-1.588652000000	-1.066748000000	-1.145365000000
O	-1.540511000000	1.204536000000	-0.184713000000
H	-0.582931000000	-0.665944000000	1.366751000000
H	-0.599590000000	-0.960142000000	-1.241861000000
O	0.583560000000	2.717467000000	0.077026000000
H	-0.268653000000	2.189381000000	0.027882000000
H	0.559878000000	3.340740000000	-0.666186000000

(H₂SO₄)₃(H₂O)

H	-1.019411000000	-0.091052000000	1.906170000000
H	0.552617000000	-0.484124000000	2.066554000000
S	1.011641000000	2.133472000000	-0.134268000000
O	-0.019773000000	1.419394000000	-0.902742000000
O	0.685458000000	2.322323000000	1.285167000000
H	0.168631000000	1.093934000000	1.988309000000
O	2.354162000000	1.548434000000	-0.380465000000
S	-2.860778000000	-0.398370000000	-0.107882000000
O	-2.144073000000	-1.304671000000	-1.185194000000
O	-2.575826000000	1.070733000000	-0.571590000000
O	-4.265123000000	-0.617434000000	-0.201088000000
O	-2.202772000000	-0.640886000000	1.185103000000
H	-1.206625000000	-1.522234000000	-0.929306000000
H	-1.582596000000	1.255575000000	-0.670992000000
S	1.679705000000	-1.813364000000	-0.084644000000
O	2.552563000000	-3.142705000000	-0.110574000000
O	2.539143000000	-0.863396000000	-0.927174000000
O	0.411949000000	-2.106532000000	-0.729436000000
O	1.662398000000	-1.403050000000	1.310488000000
H	2.277267000000	-3.684676000000	-0.874238000000
H	2.423497000000	0.180022000000	-0.676804000000
O	1.096739000000	3.644445000000	-0.653397000000
H	1.442758000000	3.641806000000	-1.565972000000
O	-0.137997000000	0.181213000000	2.379024000000

NH₃

N	0.000000000000	0.000011000000	0.000000000000
H	-0.597460000000	0.805972000000	0.000000000000
H	0.996726000000	0.114344000000	0.000000000000
H	-0.399266000000	-0.920390000000	0.000000000000

(H₂SO₄)(NH₃)

S	-0.601017000000	-0.113292000000	0.093730000000
O	0.090911000000	0.002166000000	1.357681000000
O	-1.771391000000	-0.936022000000	-0.059196000000
O	-1.024526000000	1.415627000000	-0.263719000000
O	0.415862000000	-0.471713000000	-1.031394000000
H	-1.746793000000	1.367402000000	-0.916471000000
H	1.419222000000	-0.245813000000	-0.693293000000
N	2.740920000000	0.039902000000	-0.054125000000
H	2.448314000000	0.177149000000	0.916689000000
H	3.407449000000	-0.730931000000	-0.083846000000
H	3.214781000000	0.885083000000	-0.370865000000

(H₂SO₄)₂(NH₃)

S	1.833768000000	-0.330141000000	-0.036615000000
O	2.451676000000	0.930680000000	-0.507064000000
O	1.088046000000	-0.105196000000	1.224174000000
O	3.053260000000	-1.327913000000	0.292347000000
O	1.084565000000	-1.064898000000	-1.053522000000
H	1.373107000000	2.092243000000	-0.242017000000
H	3.679973000000	-0.862585000000	0.876572000000
S	-2.116158000000	-0.150145000000	-0.007265000000
O	-1.480443000000	-0.550711000000	1.375440000000
O	-3.528149000000	-0.334639000000	0.078098000000
O	-1.548477000000	-1.198901000000	-1.028915000000
O	-1.614384000000	1.180702000000	-0.381937000000
H	-0.470755000000	-0.420106000000	1.350359000000
H	-0.536642000000	-1.145963000000	-1.075600000000
N	0.527572000000	2.725478000000	-0.039564000000
H	-0.346517000000	2.119880000000	-0.129382000000
H	0.485001000000	3.500961000000	-0.702809000000
H	0.592300000000	3.088803000000	0.912950000000

(H₂SO₄)₃(NH₃)

S	2.938705000000	0.309126000000	-0.121476000000
O	2.241578000000	1.305870000000	-1.132212000000
O	2.330982000000	0.506111000000	1.196641000000
O	2.563616000000	-1.121764000000	-0.654975000000
O	4.350160000000	0.456802000000	-0.265870000000
H	-3.305313000000	3.151894000000	0.040370000000
H	1.026836000000	-0.047789000000	2.055876000000
S	-1.613758000000	1.873119000000	-0.094021000000
O	-2.426364000000	0.956830000000	-1.023172000000
O	-1.738519000000	1.431891000000	1.290585000000
O	-0.290674000000	2.156047000000	-0.596068000000

O	-2.385544000000	3.258704000000	-0.268839000000
H	1.313337000000	1.532363000000	-0.854446000000
S	-1.140782000000	-2.095167000000	-0.143486000000
O	-1.186755000000	-3.520555000000	-0.883885000000
O	-0.037884000000	-1.305654000000	-0.716950000000
O	-2.447405000000	-1.448044000000	-0.448318000000
O	-0.963435000000	-2.468052000000	1.256230000000
H	-1.420359000000	-3.374255000000	-1.819818000000
H	1.562406000000	-1.264877000000	-0.648573000000
H	-2.400356000000	-0.093469000000	-0.746822000000
N	0.113449000000	-0.275183000000	2.532309000000
H	-0.247032000000	-1.196997000000	2.175948000000
H	-0.575411000000	0.450616000000	2.243505000000
H	0.227051000000	-0.289947000000	3.546201000000