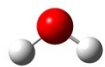
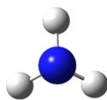


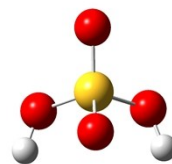
**Figure S1** Lowest Gibbs free energy structures of molecule calculated at the M06-2X/6-31+G(d,p) level.



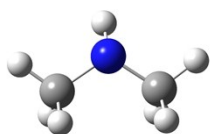
H<sub>2</sub>O



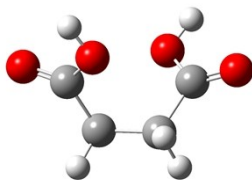
NH<sub>3</sub>



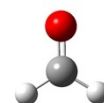
SA



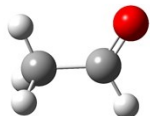
DMA



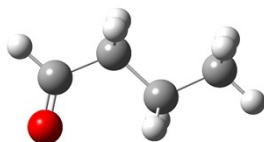
SUA



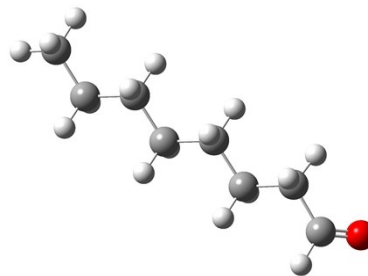
HCHO



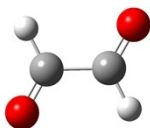
CH<sub>3</sub>CHO



CH<sub>3</sub>(CH<sub>2</sub>)<sub>2</sub>CHO



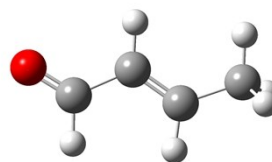
CH<sub>3</sub>(CH<sub>2</sub>)<sub>6</sub>CHO



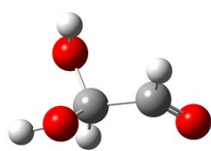
(CHO)<sub>2</sub>



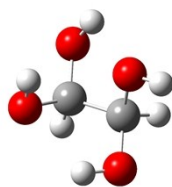
P1



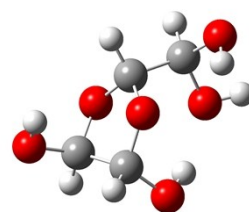
P2



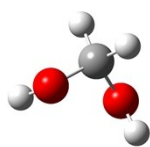
P3



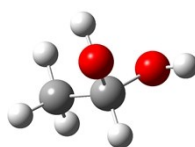
P4



P5



P6



P7



C H O N S

**Figure S1**

**Table S1** Gibbs free energy ( $G$ ) of clusters calculated at M06-2X/6-311+G(3df,3pd) level.

clusters	$G(\text{Hartree})$
SA+NH <sub>3</sub>	-756.8202
SA+SUA	-1157.1874
SA+DMA	-835.3671
SA+SA	-1400.5627
SA+HCHO	-814.7673
SA+CH <sub>3</sub> CHO	-854.0640
SA+CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> CHO	-932.6245
SA+CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> CHO	-1089.7440
SA+(CHO) <sub>2</sub>	-928.0774
SA+P1	-1007.8519
SA+P2	-931.4272
2SA+P1	-1708.1454
SA+2P1	-1315.4288
SA+P1+DMA	-1142.9487
P1+H <sub>2</sub> O	-383.9892
P1+DMA	-442.6411
P1+SUA	-764.4713
2P1	-615.1364
SA+P3	-1004.5145
SA+P4	-1080.9452
SA+P5	-1308.7645
SA+2P3	-1308.7507
SA+3P3	-1612.9834
2SA+P3	-1704.7988
3SA+P3	-2405.0846
SA+P6	-891.2000
SA+P7	-930.4888

**Table S2** Gibbs free energy ( $G$ ) of molecules calculated at the M06-2X/6-311+G(3df,3pd) level.

molecules	$G$ (Hartree)
H <sub>2</sub> O	-76.4236
NH <sub>3</sub>	-56.5352
SA	-700.2732
DMA	-135.0728
SUA	-456.8961
HCHO	-114.4901
CH <sub>3</sub> CHO	-153.7848
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> CHO	-232.3448
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> CHO	-389.4641
(CHO) <sub>2</sub>	-227.8030
P1	-307.5703
P2	-231.1465
P3	-304.2281
P4	-380.6606
P5	-608.4796
P6	-190.9174
P7	-230.2065

### Cartesian coordinates of minimum structures

H<sub>2</sub>O

O	0.00000000	0.11567100	0.00000000
H	0.76847700	-0.46256100	0.00000000
H	-0.76847700	-0.46280400	0.00000000

NH<sub>3</sub>

N	0.00000100	-0.00000700	-0.10775400
H	-0.13090000	0.93872200	0.25143300
H	-0.74752700	-0.58269300	0.25142600
H	0.87841700	-0.35598200	0.25142100

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

S	0.00018200	0.09319300	0.12648200
O	-0.00261700	-0.79873200	1.26432100
O	0.00361500	1.51796100	0.22188400
O	1.24231200	-0.30810300	-0.80119700
H	1.56883800	-1.18458600	-0.54202700
O	-1.24289000	-0.30239500	-0.80247400
H	-1.57509900	-1.17634700	-0.54196200

CH<sub>3</sub>NHCH<sub>3</sub> (DMA)

N	0.02646700	0.58649700	0.00000000
H	-0.77692800	1.20605400	0.00000000
C	0.02646700	-0.22358200	1.20696300
C	0.02646700	-0.22358200	-1.20696300
H	-0.02283500	0.42186100	2.08725200
H	0.96412500	-0.78690700	1.25757900
H	-0.80425800	-0.94923100	1.25422700
H	0.96412500	-0.78690700	-1.25757900
H	-0.02283500	0.42186100	-2.08725200
H	-0.80425800	-0.94923100	-1.25422700

HOOC(CH<sub>2</sub>)<sub>2</sub>COOH (SUA)

C	0.70396000	1.16824600	-0.29287900
C	-0.70403200	1.16823800	0.29303100
C	-1.54100800	-0.03694700	-0.06854900
C	1.54076100	-0.03719600	0.06825700
O	2.55340000	-0.36297300	-0.49725400
O	-1.05187900	-0.71123600	-1.12992400
O	-2.55330900	-0.36319800	0.49729400
O	1.05199200	-0.71131900	1.12990400
H	1.25294800	2.04768000	0.06112200
H	0.69067500	1.21979700	-1.38346400
H	-1.25291200	2.04785600	-0.06067600
H	-0.69074100	1.21941900	1.38363500
H	-1.64538800	-1.45954400	-1.29638400
H	1.64570400	-1.45944700	1.29644700

HCHO

C	-0.52446900	-0.00000200	-0.00001300
O	0.66947200	-0.00002000	0.00000300
H	-1.10463600	-0.93790100	0.00002600
H	-1.10432600	0.93807300	0.00002600

CH<sub>3</sub>CHO

C	-1.16624900	-0.14795600	-0.00006700
C	0.23266300	0.40151300	-0.00019700
O	1.22960400	-0.27896400	0.00004300
H	-1.70535000	0.22374800	-0.87789300
H	-1.70133000	0.21659500	0.88328000
H	-1.14624600	-1.23823200	-0.00432800
H	0.31761200	1.50826100	0.00017600

CH<sub>3</sub>(CH<sub>2</sub>)<sub>2</sub>CHO

C	-2.29937600	-0.06719800	-0.00040300
C	-0.82532400	-0.46498700	0.00057000

C	0.09411600	0.74920200	0.00042100
C	1.56142600	0.40766500	-0.00035000
O	1.99708000	-0.71872300	-0.00011500
H	-2.94712900	-0.94782200	-0.00058600
H	-2.54630400	0.52926300	-0.88513900
H	-2.54762100	0.53026400	0.88335500
H	-0.59722200	-1.08469500	-0.87304800
H	-0.59821200	-1.08410200	0.87474300
H	-0.09063100	1.39292600	0.87353400
H	-0.09209400	1.39269500	-0.87236400
H	2.25751900	1.27316000	-0.00100100

CH<sub>3</sub>(CH<sub>2</sub>)<sub>6</sub>CHO

C	-4.92115700	0.24163100	-0.08972200
C	-3.61882500	-0.55526300	-0.05808500
C	-2.38253300	0.34013600	-0.00329500
C	-1.07151100	-0.44291400	0.02474300
C	0.16189500	0.45548600	0.08317400
C	1.47190000	-0.32995400	0.10110100
C	2.70247600	0.58330900	0.14926600
C	3.97585100	-0.21349300	0.24907700
O	4.90533300	-0.12133200	-0.51608800
H	-4.95505600	0.89797500	-0.96574900
H	-5.01467100	0.87183400	0.80099800
H	-5.79451200	-0.41531900	-0.12892100
H	-3.55828800	-1.19941400	-0.94484300
H	-3.61679700	-1.22596100	0.81091600
H	-2.44084300	0.98423200	0.88559900
H	-2.38437000	1.01406600	-0.87171500
H	-1.01259400	-1.08348000	-0.86625600
H	-1.07080000	-1.11910900	0.89129500
H	0.10878600	1.09163700	0.97769800
H	0.15919600	1.13501800	-0.78002400
H	1.52746400	-0.96783000	-0.79021200



H	1.47937500	-1.00334400	0.96926800
H	2.63945600	1.22349000	1.04112600
H	2.76173000	1.22868600	-0.73211200
H	4.02067300	-0.93544900	1.09407600

(CHO)<sub>2</sub>

C	0.65239200	-0.39332800	0.00015200
C	-0.65279800	0.39439600	0.00035100
O	1.71532900	0.17131500	-0.00025300
O	-1.71468900	-0.17227200	-0.00029600
H	0.54369600	-1.49434700	0.00086300
H	-0.54638500	1.49560100	0.00050500

P1

C	1.67726700	-0.54872700	0.09735300
C	0.23615300	-0.95939500	0.23867700
O	2.03238900	0.53046600	-0.32269600
C	-0.74385600	0.08247600	-0.30059100
C	-2.18368700	-0.37099700	-0.14170900
O	-0.60878000	1.30308300	0.40424300
H	2.43582900	-1.29527300	0.40668800
H	0.04501400	-1.13742700	1.30731800
H	0.11005700	-1.92904600	-0.26251900
H	-0.52520900	0.24284500	-1.36742800
H	-2.36117600	-1.30815900	-0.67736600
H	-2.85850400	0.39315300	-0.53366200
H	-2.41298600	-0.51958200	0.91808100
H	0.26285100	1.66495400	0.19412900

P2

C	1.53049000	0.48849200	-0.09303100
C	2.97431000	0.55349800	0.06074100
C	3.71963800	-0.55918800	-0.07023400
C	5.20362000	-0.63507000	0.06262600

O	0.79839500	1.47585800	0.02128900
H	1.09189400	-0.49854300	-0.31596400
H	3.41326700	1.52309200	0.28267000
H	3.20530300	-1.49551200	-0.29238100
H	5.65091600	-1.02345700	-0.86079900
H	5.48074200	-1.33825300	0.85781900
H	5.64770400	0.33801900	0.28473500

P3

C	0.96183500	-0.06644100	0.37143200
C	-0.38728400	-0.00123200	-0.33666200
O	2.01584900	-0.00810000	-0.20289600
O	-1.09277200	-1.12063000	0.11435800
O	-1.04084800	1.19551800	-0.01574900
H	0.89643100	-0.15054700	1.47777600
H	-0.23832100	0.00984600	-1.42031000
H	-1.92906100	-1.18287100	-0.36395400
H	-1.23419200	1.19531400	0.93216900

P4

C	0.68300900	0.31043000	-0.43192900
C	-0.70330000	-0.34041600	-0.40882200
O	1.69357000	-0.63771100	-0.38568600
O	0.68631400	1.15053600	0.71021400
O	-0.76470400	-1.22014300	0.69004000
O	-1.70103800	0.62791400	-0.39487500
H	0.83150100	0.89803000	-1.34403200
H	-0.84720500	-0.96079600	-1.29514200
H	1.56155200	1.54301200	0.80994300
H	-1.41291500	1.35108100	0.18068100
H	-0.73712000	-0.68935500	1.49880000
H	1.41279100	-1.32682000	0.23671600

P5

C	-0.33280400	-0.91292400	0.12440800
O	0.57579300	-0.80253100	-0.93873000
C	1.69470500	-0.05848600	-0.49255200
C	1.07267600	0.85504600	0.57427700
O	0.10070200	-0.02455400	1.14246100
C	-1.74802200	-0.55145800	-0.33171200
H	1.77887100	1.12352900	1.36105700
O	2.70863800	-0.86651000	0.01445600
O	-1.68516300	0.68961800	-0.99688600
O	-2.59676400	-0.50234700	0.76951500
H	-0.34980100	-1.92615300	0.54597200
H	2.10558000	0.48315200	-1.34314300
O	0.52779000	2.02009300	0.07675000
H	-2.13770700	-1.32552300	-1.00129700
H	2.40416300	-1.29797900	0.82429300
H	-2.58792700	1.01032900	-1.11521300
H	-2.16178300	0.04036600	1.44602300
H	-0.21869200	1.78906400	-0.50475800

P6

H	0.00018600	1.15951300	0.89701800
C	0.00016600	0.53216000	0.00010200
O	1.16045400	-0.24702800	-0.09406900
O	-1.16041700	-0.24702700	0.09401600
H	0.00009700	1.16046100	-0.89628400
H	1.23449500	-0.78105800	0.70626400
H	-1.23607200	-0.77943300	-0.70718000

P7

C	-1.40013400	-0.03300400	-0.08376500
C	0.04541700	-0.00261200	0.36498500
O	0.66911600	-1.14200900	-0.17558800
O	0.71102200	1.17111300	-0.03097100
H	-1.92694100	0.84402300	0.29718500

H	-1.89149600	-0.93868700	0.27748700
H	-1.44301600	-0.03378500	-1.17815800
H	0.12167300	-0.00164900	1.45911900
H	1.59368400	-1.13798900	0.10074200
H	0.63329600	1.24895600	-0.99122900

(SA)(NH<sub>3</sub>)

N	-2.71761100	0.04247500	-0.05227200
H	-2.43377200	0.05102800	0.92717100
H	-3.15393200	0.93392600	-0.26789600
H	-3.40787500	-0.69079200	-0.18378000
S	0.59694500	-0.11725400	0.08791900
O	-0.40541300	-0.39430500	-1.07232100
O	1.01594800	1.42158000	-0.16192600
H	-1.39912000	-0.20348200	-0.73941400
H	1.74965400	1.44233900	-0.79616900
O	1.77712600	-0.92118100	-0.10756900
O	-0.12301000	-0.10038000	1.34422700

(SA)(SUA)

S	-2.34175000	-0.24414000	-0.02213500
O	-1.93274000	-0.04091900	1.48793800
O	-1.35223400	-1.38067300	-0.52798700
H	-1.06319500	0.43804000	1.51154200
H	-0.44951000	-1.04951600	-0.72330300
O	-2.02827400	0.98387700	-0.74536600
O	-3.65933000	-0.79771900	-0.05216300
C	2.52289100	1.43430800	-0.09724500
C	3.07746100	0.12431300	0.44599300
C	2.38624900	-1.06482100	-0.17205700
C	1.03175700	1.50533800	0.12167900
O	0.49211100	0.96717900	1.08015200
O	2.95215000	-2.22158800	0.16930000
O	1.41371700	-1.00265000	-0.89827100

O	0.39236700	2.18260900	-0.80456600
H	2.72283900	1.55072700	-1.16420500
H	2.98362100	2.28053500	0.42301200
H	2.92310400	0.05084000	1.52767600
H	4.15221500	0.03489700	0.26663700
H	2.44331800	-2.94369600	-0.23373900
H	-0.57668000	2.02865700	-0.71596200

(SA)(DMA)

S	1.22476500	0.26051000	0.03014400
O	2.04841700	1.36514400	0.40785300
O	0.50808500	0.36390400	-1.22356200
O	0.30925600	-0.18269400	1.10329300
O	2.21284800	-0.97634400	-0.19740000
H	3.00891200	-0.81622900	0.32104900
H	-1.57655600	1.80694500	-0.29549900
N	-1.90366700	-0.24543400	-0.17285300
H	-1.03660400	-0.31886400	0.49042500
C	-2.40487000	1.13965400	-0.07603500
C	-2.91341300	-1.28217000	0.08422900
H	-1.44358800	-0.36008700	-1.07985000
H	-3.21334300	1.29216400	-0.78686100
H	-2.76175500	1.30948800	0.93609400
H	-3.30045000	-1.15143000	1.09110700
H	-3.72681000	-1.19382500	-0.63207200
H	-2.44915600	-2.25989600	-0.00115000

(SA)<sub>2</sub>

S	-2.04517800	0.06671500	0.12479200
O	-1.46679500	0.96387400	-1.02629900
O	-2.13080000	-1.38169500	-0.54813400
H	-0.50564500	0.74843200	-1.16836200
H	-2.90494900	-1.42971000	-1.13387100
O	-3.36250000	0.54337100	0.42528500

O	-1.04491900	-0.09359100	1.16600500
S	2.04515900	-0.06674800	-0.12478200
O	2.13093000	1.38177100	0.54786200
O	1.46694000	-0.96369800	1.02656400
H	2.90541400	1.43002600	1.13313500
H	0.50587200	-0.74813700	1.16884300
O	3.36241200	-0.54347300	-0.42545800
O	1.04468400	0.09343200	-1.16581400

(SA)(HCHO)

S	0.90512300	0.10269000	-0.11841100
O	2.18443200	-0.04285000	-0.75739100
O	0.04007600	1.23663600	-0.34331800
O	1.13120100	0.07262800	1.47369200
O	0.09449200	-1.22177300	-0.37418000
H	-0.87907900	-1.05287300	-0.20068000
H	1.89054500	-0.49773500	1.67514800
C	-2.88833200	0.47186500	-0.00468000
O	-2.44623600	-0.65676500	0.06574300
H	-3.96172100	0.64865200	0.16373000
H	-2.23344700	1.32471000	-0.23190700

(SA)(CH<sub>3</sub>CHO)

S	-1.38387500	-0.12628000	-0.12043700
O	-0.45550800	-1.18722900	-0.43596000
O	-2.68379500	-0.02736600	-0.72840300
O	-0.66586200	1.25754200	-0.29302700
O	-1.58526600	-0.22355400	1.47422200
H	-2.38248500	0.27190000	1.72159300
H	0.33246500	1.14785000	-0.14250800
C	3.88585200	-0.34800300	0.06252400
C	2.41489600	-0.15900000	-0.09776000
O	1.87118200	0.92219400	0.06353000
H	4.30096300	-0.72944900	-0.87652100

H	4.06773000	-1.11525900	0.82248500
H	4.37017200	0.58780500	0.34085400
H	1.80265600	-1.03305400	-0.37038700

(SA)(CH<sub>3</sub>(CH<sub>2</sub>)<sub>2</sub>CHO)

S	2.39214400	0.09281000	-0.06549100
O	3.72082300	-0.02591800	-0.60431400
O	1.58950000	1.28314900	-0.22801300
O	2.47841100	-0.12192800	1.52869600
O	1.56979100	-1.15577700	-0.53572000
H	0.57441700	-0.98069100	-0.41316100
H	3.19650100	-0.74526100	1.72325800
C	-5.20364900	-0.10142300	0.17717200
C	-3.72913700	-0.47603300	0.05000100
C	-2.83982900	0.75669700	-0.04994500
C	-1.38044200	0.46514000	-0.18808700
O	-0.93832800	-0.67330200	-0.23190600
H	-5.83113600	-0.99316400	0.24898900
H	-5.54031500	0.47516200	-0.69062900
H	-5.38134900	0.50567000	1.07093900
H	-3.57016300	-1.10368500	-0.83296400
H	-3.41340900	-1.07584700	0.90990300
H	-2.95175400	1.41277900	0.82634200
H	-3.11724600	1.38799100	-0.90777400
H	-0.68310000	1.31599700	-0.25183200

(SA)(CH<sub>3</sub>(CH<sub>2</sub>)<sub>6</sub>CHO)

C	7.95596100	-0.43690500	0.11355100
C	6.54813400	-0.89703900	-0.25836600
C	5.47152200	0.09409500	0.17958800
C	4.05802700	-0.35001600	-0.19173700
C	2.98598200	0.64415400	0.24880900
C	1.57365900	0.20002800	-0.12799900
C	0.51319400	1.21918400	0.31433600

C	-0.86690500	0.73113400	0.01869000
O	-1.67637100	1.37839700	-0.62842200
H	8.05212300	-0.31091900	1.19712100
H	8.18771600	0.52544400	-0.35475000
H	8.71265300	-1.15747200	-0.20877700
H	6.34580400	-1.87432400	0.19846500
H	6.48174300	-1.04419800	-1.34407200
H	5.67496200	1.07435200	-0.27412600
H	5.53366400	0.23952600	1.26738900
H	3.85428700	-1.33021000	0.26125000
H	3.99626400	-0.49327100	-1.27947200
H	3.19013700	1.62476700	-0.20206600
H	3.04284100	0.78481800	1.33712800
H	1.36210300	-0.77445500	0.33110300
H	1.51184600	0.05749000	-1.21401400
H	0.65934600	2.19314200	-0.16110400
H	0.58110100	1.35170300	1.40401200
H	-1.15594900	-0.26199400	0.40273200
S	-4.43584100	-0.52550000	0.01322900
O	-5.59507100	-1.24601100	-0.44187500
O	-3.24098700	-1.18887700	0.48111500
O	-4.88051800	0.41510900	1.24361100
O	-4.05529700	0.51599300	-1.09506300
H	-3.11492300	0.86837400	-0.92808600
H	-5.79374600	0.71053300	1.09943500

(SA)((CHO)<sub>2</sub>)

S	-1.38780300	-0.26878000	-0.00970300
O	-2.50106900	-1.05845100	0.43588400
O	-0.18036800	-0.84384000	-0.55146300
O	-1.89404700	0.75710600	-1.13281600
O	-1.00818900	0.69661100	1.18748100
H	-0.14699800	1.14009100	0.99216800
H	-2.81840000	0.99722200	-0.95546700



C	2.20186900	0.87594900	-0.25240100
C	2.42497600	-0.53151200	0.29204100
O	1.37614700	1.62779700	0.21438000
O	3.30319300	-1.20771700	-0.17404900
H	2.86842100	1.17430600	-1.07963100
H	1.77542100	-0.84978900	1.12500300

(SA)(P1)

S	-1.79868500	-0.17883700	-0.03524700
O	-3.21902800	-0.31068200	-0.22197800
O	-0.92214600	-1.31910900	0.10343200
O	-1.56116500	0.67030400	1.32621800
O	-1.24138300	0.78609900	-1.12696000
H	-0.20871200	0.69794900	-1.19606600
H	-2.31779800	1.26311700	1.46061900
C	1.86618600	-1.60263600	0.57440300
C	1.78372000	-0.16318600	1.01183700
O	2.19974600	-1.93842100	-0.54258800
C	2.05760400	0.82319100	-0.12166700
C	1.74751600	2.25328300	0.27439400
O	1.25054700	0.51661900	-1.27355700
H	1.61442600	-2.36533100	1.33256500
H	2.51693700	-0.01516000	1.81695700
H	0.79631600	0.00240200	1.46040300
H	3.10454600	0.73432000	-0.43460100
H	1.94541000	2.93020200	-0.55958800
H	2.36501700	2.55253700	1.12556700
H	0.69529500	2.34482700	0.56318200
H	1.48479500	-0.38587500	-1.55542900

(SA)(P2)

S	-2.22223000	-0.25441100	-0.11357000
O	-1.11880200	-1.14886000	-0.38226900
O	-3.51216000	-0.41384400	-0.73222700

O	-1.76107900	1.22386100	-0.33014200
O	-2.42564400	-0.33421200	1.48342800
H	-3.29236900	0.04083000	1.70677100
H	-0.74908200	1.30873800	-0.17742100
C	1.49335200	0.44987300	-0.07014700
C	2.94019900	0.55217400	0.05862900
C	3.69221300	-0.55328900	-0.05464700
C	5.17954400	-0.59749900	0.04647400
O	0.74977500	1.42361000	0.01729100
H	1.06401900	-0.54814600	-0.25444000
H	3.36519100	1.53634700	0.23965000
H	3.18474300	-1.50227600	-0.23694800
H	5.60861500	-1.00319000	-0.87576400
H	5.48434100	-1.26660700	0.85795300
H	5.60164900	0.39287800	0.22680400

(SA)<sub>2</sub>(P1)

S	0.79777900	2.05238000	0.21221300
O	0.26902900	1.00221400	1.11072000
O	1.19337200	3.31051300	0.76229200
O	-0.30737000	2.32197600	-0.88558800
O	1.98609700	1.42785800	-0.57497100
H	1.75743400	0.46058200	-0.89854100
H	-0.72057700	1.47203100	-1.17811600
S	-2.53093900	-0.38069600	-0.28536500
O	-3.79102100	0.04530000	-0.80773400
O	-1.31260700	-0.20646400	-1.09898800
O	-2.66725000	-1.90340600	0.08939800
O	-2.25090800	0.30463700	1.10298700
H	-1.29719700	0.61545900	1.16806600
H	-1.82588300	-2.21240700	0.50161200
C	0.76057200	-1.69265200	1.52384600
C	2.16504200	-1.52602000	1.02981900
O	-0.11093300	-2.17272300	0.82081700

C	2.29476500	-1.81918500	-0.46380000
C	3.71257300	-1.62321100	-0.96524700
O	1.45645400	-0.92354100	-1.21662500
H	0.53444700	-1.37668500	2.55530500
H	2.80813300	-2.19928900	1.61386900
H	2.49081900	-0.50465100	1.26636400
H	1.95393000	-2.83944100	-0.66838300
H	4.04308800	-0.59435200	-0.78982100
H	3.76303000	-1.82782000	-2.03645600
H	4.39613400	-2.29946400	-0.44528900
H	0.51059800	-1.12540900	-1.08432700

(SA)(P1)<sub>2</sub>

S	-0.00002700	-1.16621200	-0.00010100
O	1.25159300	-1.87496500	0.15596200
O	-1.25175500	-1.87477500	-0.15616000
O	0.10995800	-0.17766500	-1.22703100
O	-0.10987200	-0.17766100	1.22683700
H	-1.06484800	0.20065900	1.27737400
H	1.06491500	0.20070200	-1.27745000
C	-3.93060300	-0.91378300	-0.59820500
C	-3.22687300	0.35341900	-1.00344400
O	-4.39052200	-1.09504600	0.51031600
C	-3.05025700	1.34106000	0.14956800
C	-2.12262400	2.48180800	-0.22096800
O	-2.48954900	0.69153200	1.30440300
H	-4.02580500	-1.69470100	-1.37346800
H	-3.81684000	0.82076600	-1.80453500
H	-2.26278000	0.08096600	-1.45009900
H	-4.03104100	1.73088300	0.44829400
H	-1.98849400	3.15567300	0.62860300
H	-2.53837200	3.04949700	-1.05799300
H	-1.14812200	2.08656900	-0.52643700
H	-3.10057200	-0.02601400	1.55118900

C	3.93039100	-0.91394000	0.59827800
C	3.22675500	0.35329900	1.00354900
O	4.39047400	-1.09511200	-0.51019000
C	3.05036800	1.34099800	-0.14943700
C	2.12287300	2.48187600	0.22105000
O	2.48965800	0.69154500	-1.30431200
H	4.02535200	-1.69497000	1.37345800
H	3.81671300	0.82053800	1.80471300
H	2.26258800	0.08093300	1.45010000
H	4.03123300	1.73067900	-0.44808000
H	1.98892900	3.15579300	-0.62850900
H	2.53862700	3.04946800	1.05813800
H	1.14828300	2.08677200	0.52641100
H	3.10062200	-0.02606600	-1.55105000

(SA)(P1)(DMA)

S	1.61926000	-0.96594000	-0.03528000
O	2.12886000	0.03485000	-1.00732900
O	0.72819000	-1.95742900	-0.66582500
O	1.09021600	-0.34512300	1.18382600
O	2.91116000	-1.79475000	0.47913200
H	3.22698500	-2.34519900	-0.25367200
H	-0.37083500	1.43277400	-0.13259900
C	-1.46953700	0.14573800	1.87905500
C	-1.96290100	-1.00044300	1.04232400
O	-1.52739900	1.31249500	1.54160500
C	-2.41236300	-0.60023400	-0.36120100
C	-3.03611800	-1.77600300	-1.10101200
O	-1.32032500	-0.06671600	-1.10663000
H	-1.05763400	-0.12129200	2.86881900
H	-1.15818500	-1.74659300	0.99111300
H	-2.79003200	-1.46914100	1.59557900
H	-3.13314300	0.22121200	-0.28522300
H	-3.32958000	-1.47202100	-2.10867600

H	-2.31281700	-2.59536700	-1.18121300
H	-3.92069600	-2.14783200	-0.57501700
H	-0.68012000	-0.79165700	-1.24489900
N	0.38670100	2.06436500	-0.44268700
C	0.91978900	2.81556400	0.71591900
C	-0.14167700	2.90144600	-1.53908500
H	1.12672000	1.41211100	-0.79604300
H	1.29017600	2.08595400	1.43613300
H	0.11334300	3.40119000	1.15767200
H	1.72779200	3.46377900	0.37270300
H	0.66326700	3.51712000	-1.94281600
H	-0.93707200	3.53651300	-1.14580300
H	-0.54202000	2.23991900	-2.30699700

(P1)(H<sub>2</sub>O)

O	-1.60506900	1.92639100	-0.27428600
H	-2.20011700	2.60424000	0.05720300
H	-1.32904000	1.38375600	0.48501900
C	1.85092800	0.28300400	-0.56037700
C	0.51971500	-0.28327600	-0.96652700
O	2.26545600	0.28656800	0.57979300
C	-0.21310800	-0.98146000	0.17921300
C	-1.57335500	-1.49476200	-0.25611700
O	-0.42908200	-0.07664400	1.26315800
H	2.46639600	0.72413200	-1.36861000
H	0.68415700	-0.97399800	-1.80469300
H	-0.08984100	0.54581600	-1.35728600
H	0.40440500	-1.81644400	0.53936600
H	-1.46812300	-2.22769600	-1.06119400
H	-2.18633500	-0.66192200	-0.61482300
H	-2.08020200	-1.96989100	0.58701700
H	0.44317800	0.16045700	1.61152800

(P1)(DMA)

C	0.99201600	1.84055400	-0.09206800
C	1.55187400	0.58241000	-0.69605000
O	-0.06668400	2.33461900	-0.41098100
C	1.78711600	-0.46800800	0.40584400
C	2.14471600	-1.82207700	-0.19687800
O	0.66736000	-0.55450100	1.25481000
H	1.60533600	2.30983700	0.70363600
H	2.50325000	0.81623900	-1.19163500
H	0.84985600	0.20948200	-1.45058100
H	2.61879800	-0.12697300	1.03738400
H	1.31576800	-2.18517000	-0.81512400
H	2.31687200	-2.54668300	0.60237600
H	3.04275300	-1.76088500	-0.82059200
H	-0.15815500	-0.56536700	0.70418600
N	-1.68614400	-0.21499400	-0.17479000
C	-2.54549600	0.20791000	0.92889400
C	-2.27553300	-1.28681200	-0.96753600
H	-1.48391700	0.59521800	-0.75813700
H	-2.08337300	1.05777100	1.43630400
H	-2.63828500	-0.61288200	1.64710200
H	-3.55471700	0.49412800	0.59685700
H	-3.26977900	-1.03150000	-1.36506100
H	-2.37831100	-2.17945400	-0.34253700
H	-1.61665600	-1.53361500	-1.80452000

(P1)(SUA)

C	-1.03226400	1.83874800	-0.40538900
C	-1.54344900	0.99685100	0.73458600
O	-1.64571800	1.99782800	-1.43864600
C	-2.80874500	0.22352200	0.37219300
C	-3.26845500	-0.68476900	1.49693600
O	-2.57887400	-0.61025800	-0.77136900
H	-0.05418100	2.33017300	-0.24938800
H	-1.73830900	1.67186200	1.58042000

H	-0.73419800	0.33319900	1.06439100
H	-3.60241500	0.93645000	0.11516200
H	-4.16609500	-1.23077100	1.19773000
H	-3.49432300	-0.09993300	2.39292400
H	-2.48446900	-1.40833200	1.74348900
H	-2.33720900	-0.02848500	-1.51049600
C	1.90042900	-1.79729000	-0.02603000
C	2.98136600	-0.75104600	-0.23205000
C	2.67099000	0.52196400	0.51473500
C	0.57275100	-1.32360800	-0.57419900
O	0.45487300	-0.35737100	-1.30244600
O	3.57418500	1.48371800	0.26036600
O	1.74057400	0.69018000	1.26950200
O	-0.44823900	-2.06778400	-0.16998500
H	1.76567300	-2.03548100	1.03249200
H	2.16208600	-2.73054800	-0.53559600
H	3.08813600	-0.49230700	-1.28953700
H	3.95642700	-1.11007500	0.11299500
H	3.32142500	2.26755800	0.77198400
H	-1.29268700	-1.64004300	-0.49063000

(P1)<sub>2</sub>

C	-1.72646100	1.62035000	-0.81925800
C	-2.05184700	0.71805700	0.33707400
O	-0.71923000	2.28611400	-0.90361500
C	-2.28568200	-0.71321400	-0.17105600
C	-2.58814600	-1.67396800	0.97196200
O	-1.17487900	-1.14021300	-0.93389500
H	-2.47342300	1.64180400	-1.63994300
H	-2.96201600	1.09082900	0.82656500
H	-1.22653300	0.75157400	1.05775000
H	-3.13301200	-0.70264200	-0.86906600
H	-1.74029000	-1.71499500	1.66480600
H	-2.75547600	-2.67880900	0.57715500

H	-3.47537000	-1.36052900	1.53040200
H	-0.42751200	-1.28058300	-0.32127600
C	1.66031800	1.64033000	0.51543400
C	1.93723600	0.59416400	-0.53263400
O	1.45560800	1.37636900	1.68452900
C	2.15906800	-0.80365900	0.04180900
C	2.35086100	-1.83962100	-1.05075200
O	1.03007400	-1.21390200	0.81623300
H	1.64910500	2.68936900	0.17500100
H	2.80766900	0.91678400	-1.11900800
H	1.08151200	0.59459800	-1.22316900
H	3.04169000	-0.78648100	0.69664900
H	1.47151700	-1.86700000	-1.70281800
H	2.48774600	-2.82901800	-0.60834100
H	3.22794000	-1.60073000	-1.65868500
H	0.96178200	-0.58575400	1.55248300

(SA)(P3)

S	1.91355800	0.07504600	-0.00920800
O	3.24771600	0.32103900	-0.47917000
O	1.02972700	1.14793900	0.40105400
O	1.98318300	-0.87791500	1.28133300
O	1.18498000	-0.81970800	-1.06867300
H	0.19578400	-0.87009200	-0.85226300
H	2.72924500	-1.49233000	1.18620700
C	-3.32688200	0.14439400	0.41064400
C	-1.81209600	0.30378600	0.29924600
O	-3.88742000	-0.80956900	-0.06747400
O	-1.28846700	-0.84334700	-0.34140100
O	-1.61840400	1.47007000	-0.41794800
H	-3.86788000	0.96481700	0.91001300
H	-1.34261600	0.35219000	1.28949400
H	-2.01337900	-1.29772600	-0.80596400
H	-0.69472300	1.74525600	-0.30128200



(SA)(P4)

S	2.28388800	-0.11342500	-0.08294000
O	1.36261000	-1.08724800	-0.63356500
O	3.67072900	-0.08685700	-0.45216400
O	2.16683000	-0.33682200	1.50557800
O	1.70347500	1.32730100	-0.27088400
H	0.69461600	1.32583200	-0.11988600
H	2.91148900	0.10297000	1.94756300
C	-1.40370200	-0.09377200	0.20828900
C	-2.89119900	0.05612700	0.54399000
O	-0.81776400	1.19932800	0.16963100
O	-1.36222400	-0.72131800	-1.03324300
O	-3.43922200	1.01748200	-0.33464700
O	-3.52673500	-1.17254400	0.47664000
H	-0.85641600	-0.65522100	0.97178800
H	-3.02294800	0.46035100	1.54930500
H	-0.45269500	-1.01938300	-1.20111500
H	-3.12897700	-1.67696300	-0.24924300
H	-3.53646800	0.60784900	-1.20587600
H	-1.44297000	1.78064500	-0.29794800

(SA)(P5)

S	2.45438800	-0.15693900	-0.01541400
O	3.83734000	-0.48692500	-0.15920100
O	1.58581000	-0.96836500	0.83833100
O	1.78815400	-0.13266200	-1.45674900
O	2.36562000	1.34562000	0.44597900
H	1.40910400	1.61960200	0.51864100
H	0.82202100	-0.32315400	-1.37612200
C	-1.80204600	0.43887700	-0.76040300
O	-0.84710200	-0.58020100	-0.98488400
C	-1.21440600	-1.72166100	-0.19823200
C	-1.83727800	-1.03225500	1.02148700

O	-2.52405300	0.05223500	0.39770400
C	-1.13399300	1.79871500	-0.52722400
H	-2.59710700	-1.63199300	1.52537800
O	-2.09397500	-2.55402500	-0.85944000
O	-0.24701400	1.74041600	0.56370300
O	-2.12169600	2.75939200	-0.36052800
H	-2.50213000	0.51532900	-1.59979700
H	-0.30153600	-2.28050400	0.00746000
O	-0.90804500	-0.57361900	1.94494800
H	-0.54394300	2.09263200	-1.39896400
H	-2.96631400	-2.14031700	-0.92008600
H	-0.63987600	1.23195200	1.30081100
H	-2.71223400	2.48297600	0.35538700
H	0.00782800	-0.77247900	1.66124000

(SA)(P3)<sub>2</sub>

S	-0.00002700	-1.16621200	-0.00010100
O	1.25159300	-1.87496500	0.15596200
O	-1.25175500	-1.87477500	-0.15616000
O	0.10995800	-0.17766500	-1.22703100
O	-0.10987200	-0.17766100	1.22683700
H	-1.06484800	0.20065900	1.27737400
H	1.06491500	0.20070200	-1.27745000
C	-3.93060300	-0.91378300	-0.59820500
C	-3.22687300	0.35341900	-1.00344400
O	-4.39052200	-1.09504600	0.51031600
C	-3.05025700	1.34106000	0.14956800
C	-2.12262400	2.48180800	-0.22096800
O	-2.48954900	0.69153200	1.30440300
H	-4.02580500	-1.69470100	-1.37346800
H	-3.81684000	0.82076600	-1.80453500
H	-2.26278000	0.08096600	-1.45009900
H	-4.03104100	1.73088300	0.44829400
H	-1.98849400	3.15567300	0.62860300

H	-2.53837200	3.04949700	-1.05799300
H	-1.14812200	2.08656900	-0.52643700
H	-3.10057200	-0.02601400	1.55118900
C	3.93039100	-0.91394000	0.59827800
C	3.22675500	0.35329900	1.00354900
O	4.39047400	-1.09511200	-0.51019000
C	3.05036800	1.34099800	-0.14943700
C	2.12287300	2.48187600	0.22105000
O	2.48965800	0.69154500	-1.30431200
H	4.02535200	-1.69497000	1.37345800
H	3.81671300	0.82053800	1.80471300
H	2.26258800	0.08093300	1.45010000
H	4.03123300	1.73067900	-0.44808000
H	1.98892900	3.15579300	-0.62850900
H	2.53862700	3.04946800	1.05813800
H	1.14828300	2.08677200	0.52641100
H	3.10062200	-0.02606600	-1.55105000

(SA)<sub>2</sub>(P3)

S	0.79777900	2.05238000	0.21221300
O	0.26902900	1.00221400	1.11072000
O	1.19337200	3.31051300	0.76229200
O	-0.30737000	2.32197600	-0.88558800
O	1.98609700	1.42785800	-0.57497100
H	1.75743400	0.46058200	-0.89854100
H	-0.72057700	1.47203100	-1.17811600
S	-2.53093900	-0.38069600	-0.28536500
O	-3.79102100	0.04530000	-0.80773400
O	-1.31260700	-0.20646400	-1.09898800
O	-2.66725000	-1.90340600	0.08939800
O	-2.25090800	0.30463700	1.10298700
H	-1.29719700	0.61545900	1.16806600
H	-1.82588300	-2.21240700	0.50161200
C	0.76057200	-1.69265200	1.52384600

C	2.16504200	-1.52602000	1.02981900
O	-0.11093300	-2.17272300	0.82081700
C	2.29476500	-1.81918500	-0.46380000
C	3.71257300	-1.62321100	-0.96524700
O	1.45645400	-0.92354100	-1.21662500
H	0.53444700	-1.37668500	2.55530500
H	2.80813300	-2.19928900	1.61386900
H	2.49081900	-0.50465100	1.26636400
H	1.95393000	-2.83944100	-0.66838300
H	4.04308800	-0.59435200	-0.78982100
H	3.76303000	-1.82782000	-2.03645600
H	4.39613400	-2.29946400	-0.44528900
H	0.51059800	-1.12540900	-1.08432700

(SA)<sub>2</sub>(P3)<sub>2</sub>

S	0.35700300	2.10583000	0.28790600
O	0.15269500	1.16231300	-0.79947200
O	1.60702700	2.82344900	0.37122100
O	0.11494400	1.36616700	1.65476900
O	-0.77798800	3.19837700	0.27086000
H	-1.65164000	2.73260200	0.27660400
H	-0.33324200	0.48431700	1.50558000
S	-0.44525400	-2.08040600	0.73324400
O	-1.18291900	-0.87120300	1.15240700
O	0.45054100	-2.67868900	1.67995800
O	0.26027000	-1.76491600	-0.62678600
O	-1.49450900	-3.15032900	0.26908300
H	-2.11207100	-2.75362200	-0.39192900
H	1.11457700	-1.21973600	-0.44183100
C	-2.55701200	-0.34013700	-1.25913300
C	-3.40151100	0.88360400	-0.89747400
O	-3.05470900	-1.44815000	-1.19318100
O	-4.72232700	0.54732600	-0.73111500
O	-2.82704300	1.43802800	0.27872300

H	-1.49637900	-0.17494400	-1.49271500
H	-3.30574200	1.66811000	-1.65404500
H	-4.79132000	-0.41762700	-0.64836600
H	-2.84499700	0.78432500	0.99579000
C	4.31263000	-0.59041900	-1.28232600
C	3.21490000	0.26168800	-0.64603000
O	4.43459200	-1.75787700	-1.01388700
O	2.36311200	-0.57167700	0.12818500
O	3.88553900	1.19362300	0.11696500
H	5.00632100	-0.05904200	-1.95604100
H	2.56427500	0.71881700	-1.40212900
H	2.90619600	-1.25570100	0.55947300
H	3.26820000	1.90575700	0.35915300

(SA)(P3)<sub>3</sub>

C	-2.21291900	-1.22872600	-1.95212000
C	-1.72062300	0.17742400	-1.62122200
O	-2.48575200	-2.02319300	-1.08583900
O	-2.44020500	1.05746700	-2.41549700
O	-1.86966900	0.42672700	-0.24333600
H	-2.29767800	-1.47240000	-3.02498600
H	-0.63903800	0.23297000	-1.80337600
H	-1.98692900	1.91292900	-2.39232100
H	-2.80955700	0.42440800	-0.00336700
C	-1.49302400	-0.31283100	2.90701900
C	-0.36787900	-1.19546000	2.35841500
O	-2.57659200	-0.26475800	2.38342800
O	-0.77809600	-1.84598900	1.19335900
O	0.78442700	-0.41145700	2.18279600
H	-1.23645200	0.28641400	3.79804500
H	-0.10590400	-1.95980400	3.09837600
H	-1.57534400	-1.42024400	0.81479900
H	0.55092300	0.47538900	1.80068100
C	0.61209600	3.10677100	-0.75508600

C	0.85010900	2.79867400	0.72372100
O	-0.39190600	2.77248500	-1.33733400
O	-0.12719600	1.91502000	1.20765200
O	2.14068300	2.32340700	0.91378700
H	1.42757400	3.65428300	-1.25996000
H	0.78969600	3.73912000	1.28686600
H	-0.72964500	1.61587100	0.49055500
H	2.26500800	1.55274800	0.33343300
S	1.95267100	-1.15006000	-0.82134300
O	2.90502600	-1.49401400	-1.83320700
O	1.42412500	0.21777300	-0.75468100
O	2.56106100	-1.48557300	0.59372400
O	0.72565000	-2.13161200	-0.94782600
H	0.14848300	-2.08408000	-0.12614100
H	1.97711000	-1.08203200	1.30831300

(SA)<sub>3</sub>(P3)

S	-3.29849400	-0.18602700	0.27207400
O	-2.52718300	-0.75535700	-0.83905400
O	-4.69912500	-0.43003800	0.39812500
O	-3.08595000	1.37341400	0.24389200
O	-2.58047800	-0.64203800	1.60690000
H	-1.65885700	-0.92790400	1.40772000
H	-2.13933100	1.58366900	0.07156400
S	0.55153400	2.57547300	-0.16006400
O	-0.08121900	3.85094100	-0.06392600
O	-0.34101000	1.38028600	-0.16239100
O	1.59788800	2.38446300	0.96401100
O	1.38062200	2.53424100	-1.49920000
H	2.00774000	1.77647700	-1.49709900
H	1.83028600	1.39550300	1.17763100
S	0.24679100	-1.91052100	-0.59415500
O	-0.08583100	-1.44677500	0.76359200
O	1.49144500	-2.63555900	-0.72276400

O	0.26631700	-0.68524300	-1.55144400
O	-0.89972900	-2.81670900	-1.13948100
H	-1.74038900	-2.28409900	-1.13751500
H	-0.06913600	0.14714500	-1.07732100
C	3.44056600	-0.56493300	-0.36640500
C	3.24339000	-0.73955000	1.14327300
O	2.94111100	0.34373300	-0.98627400
O	2.11865300	0.00571300	1.58895500
O	3.19118200	-2.06399700	1.51157700
H	4.10978600	-1.29603600	-0.85134300
H	4.11432300	-0.29301600	1.63895200
H	1.31175200	-0.54563900	1.52978200
H	2.63926600	-2.56857600	0.89058300

(SA)(P6)

S	-1.22436800	-0.11408800	-0.11064300
O	-0.28692800	-1.16996400	-0.43042700
O	-2.58844400	-0.14350200	-0.55981200
O	-0.61266500	1.27054600	-0.49996500
O	-1.21464100	-0.06428500	1.49951000
H	-1.99309000	0.42692300	1.80844700
H	0.40772000	1.26555600	-0.38340600
H	1.62812500	-0.16010700	1.32174000
C	2.37426100	0.01057700	0.53887100
O	2.53120100	-1.05911700	-0.31174200
O	1.90304200	1.17834500	-0.16057400
H	3.34901600	0.23719700	0.97481400
H	1.64975600	-1.40232600	-0.53085400
H	2.45027700	1.29853300	-0.94959000

(SA)(P7)

S	1.46811400	-0.14045300	-0.13343600
O	2.76069000	-0.76319700	-0.21067900
O	0.53520500	-0.17367800	-1.24075100

O	1.66856000	1.43034300	0.16930600
O	0.75822800	-0.64611900	1.16527500
H	-0.18773600	-0.24935600	1.21857200
H	2.48520300	1.55022400	0.68076500
C	-2.41210600	-1.30223500	-0.15685300
C	-2.44239300	0.18837900	0.10263300
O	-1.54106400	0.44128500	1.20813700
O	-2.09223300	0.96896600	-0.98357400
H	-3.13780500	-1.54034700	-0.93673000
H	-2.66772800	-1.85325800	0.75079900
H	-1.41905500	-1.60821900	-0.49813200
H	-3.43588800	0.52426800	0.41329800
H	-1.46657000	1.40079500	1.31367000
H	-1.24833900	0.64548500	-1.34366000

(SA)(H<sub>2</sub>O)<sub>2</sub>

S	-0.00008800	0.44147300	-0.00038300
O	-1.09447800	1.15058500	-0.62761400
O	1.09482300	1.15259600	0.62371400
O	0.58481700	-0.54056800	-1.09084200
O	-0.58577300	-0.53519500	1.09461800
H	-1.51518200	-0.79635500	0.82503100
H	1.51477800	-0.79986400	-0.82108600
O	-2.99391200	-0.77175900	0.08548900
H	-2.87221300	0.01016200	-0.47606900
H	-3.33616800	-1.48145300	-0.46722500
O	2.99414300	-0.77157500	-0.08504200
H	3.33965800	-1.47993100	0.46735800
H	2.87357500	0.01120000	0.47554400

(SA)(NH<sub>3</sub>)(H<sub>2</sub>O)

S	0.01975300	0.38832600	-0.00252000
O	-0.95507300	1.18559300	0.71472900
O	1.08656300	1.02966400	-0.75134100



O	-0.72916600	-0.58413400	-0.96580800
O	0.68413700	-0.57669700	1.06768800
H	1.60495000	-0.81404400	0.76474000
H	-1.72652700	-0.70560900	-0.63651100
N	-3.12999700	-0.66090000	-0.03710300
H	-3.87594100	-0.50256200	-0.70752300
H	-3.38148400	-1.45945100	0.53754500
H	-3.05253400	0.15899300	0.56420000
O	3.07420000	-0.76697500	-0.06367700
H	2.84083400	-0.00570000	-0.62036000
H	3.89934900	-0.55815500	0.38522000

(SA)(P1)(H<sub>2</sub>O)

S	-2.58219900	-0.12934400	-0.15093400
O	-1.66757400	0.51725300	-1.07615100
O	-3.79948600	-0.74692100	-0.60878500
O	-2.96888700	1.04702000	0.88121600
O	-1.80727100	-1.13785100	0.73767400
H	-0.77593400	-0.85497300	0.83004000
H	-3.73449800	0.76851500	1.40847200
C	1.14932200	-1.08856600	-0.37137600
C	2.64199600	-1.27532100	-0.17385600
O	0.56214200	-0.49049500	0.78779900
C	3.42174300	0.02734900	-0.15434400
C	4.83728900	-0.03557400	0.35994400
O	2.93041700	1.07057000	-0.53956000
H	0.66567700	-2.05896300	-0.51236700
H	0.94062900	-0.46874700	-1.25004300
H	2.83782200	-1.82593200	0.75372500
H	3.05671600	-1.88373900	-0.98990900
H	4.80844200	-0.16236400	1.44786800
H	5.36447900	-0.90040800	-0.05335000
H	5.36527300	0.88661300	0.11849300
H	-0.36966400	1.94284000	-0.43051000

O	0.38868700	2.01449800	0.17110200
H	1.18178600	2.15591200	-0.36542200
H	0.56813400	0.51084400	0.66936600

(SA)(P1)(H<sub>2</sub>O)<sub>2</sub>

S	-1.50013100	0.81452200	0.10886400
O	-0.73940000	0.24711300	1.21648700
O	-1.58360800	2.26320700	0.05915400
O	-2.94673900	0.23752000	0.06787200
O	-0.92613500	0.23579800	-1.23435500
H	0.10272300	0.16730800	-1.17439000
H	-2.88070400	-0.77747000	-0.05668200
C	0.67955300	-1.88819700	0.87104400
C	1.95287900	-1.09352900	0.95219400
O	0.21436900	-2.29976100	-0.17546000
C	2.46650500	-0.61804100	-0.40312900
C	3.86493900	-0.02770700	-0.30406500
O	1.57851000	0.34868100	-0.97009400
H	0.18045800	-2.11033800	1.82943900
H	2.70160700	-1.73010200	1.44553800
H	1.77223300	-0.24236700	1.62127900
H	2.45577100	-1.45677100	-1.10527200
H	3.87553600	0.81431500	0.39757800
H	4.19196400	0.32946800	-1.28320100
H	4.57848300	-0.77665600	0.05077400
H	1.63572300	1.20540100	-0.48454000
O	1.24639900	2.72035700	0.31129200
H	1.52501900	3.54126100	-0.10711700
H	0.27890200	2.78189400	0.41148000
O	-2.56292100	-2.26061800	-0.33427200
H	-2.84683100	-2.53421600	-1.21368500
H	-1.59584700	-2.41760900	-0.29427200

(SA)<sub>2</sub>(P1)(H<sub>2</sub>O)

S	-2.80957300	-0.29324900	0.26107600
O	-1.97946000	0.73869500	-0.35943500
O	-4.15908600	0.00286800	0.62909100
O	-2.04519600	-0.80346000	1.54613200
O	-2.84019200	-1.55075000	-0.68944800
H	-1.92309700	-1.84172800	-0.91912500
H	-1.06437400	-0.82994000	1.37736600
S	0.89043200	-1.54181300	-0.37002800
O	-0.22005300	-2.25094100	-0.98580700
O	0.53416100	-0.77346100	0.84055600
O	1.59738700	-0.58393100	-1.35945400
O	2.00358100	-2.56252600	-0.05205500
H	2.87017600	-2.05598600	0.24089700
H	1.16232800	0.39139500	-1.34173100
C	1.88419500	1.45725700	1.33270500
C	0.73254800	2.34331400	0.95553600
O	2.82800400	1.24635400	0.59372100
C	0.71014100	2.72515000	-0.52094200
C	-0.31126400	3.81041500	-0.81641800
O	0.41384900	1.57133000	-1.32939000
H	1.85357200	1.00665100	2.33929800
H	0.79889500	3.24360000	1.58331800
H	-0.20175200	1.84014500	1.23829600
H	1.71044000	3.03447600	-0.83453400
H	-0.06512400	4.72613400	-0.27201900
H	-1.31224500	3.48502200	-0.51338800
H	-0.32372500	4.03235800	-1.88553100
H	-0.51109800	1.29742500	-1.15617800
O	4.00808900	-1.21468700	0.60718000
H	3.73443800	-0.27146100	0.65178800
H	4.75544100	-1.26984100	0.00076800

(SA)(P3)(H<sub>2</sub>O)

S	1.41658300	0.45535300	-0.01750000
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O	0.40161400	1.30982400	0.57030700
O	2.62716200	1.01964900	-0.57372600
O	0.75727600	-0.40665400	-1.15590600
O	1.79442100	-0.59926700	1.09068700
H	2.69307800	-0.98722700	0.86539200
H	-0.18875400	-0.64515500	-0.89945800
C	-3.81069300	-0.17393700	0.40927600
C	-2.31988900	0.14918200	0.35017100
O	-4.25602800	-1.15880900	-0.12504600
O	-1.65855600	-0.89933800	-0.32918800
O	-2.23446400	1.36619100	-0.30253700
H	-4.44828500	0.56129700	0.92717400
H	-1.88345000	0.19713300	1.35527700
H	-2.32147900	-1.40923400	-0.82706700
H	-1.35201000	1.73530300	-0.13229000
O	4.18534700	-1.16674300	0.21287500
H	4.21800500	-0.38252500	-0.35728900
H	4.46688300	-1.92552100	-0.30815600

(SA)(P3)(H<sub>2</sub>O)<sub>2</sub>

S	-0.97745800	-0.47143200	-0.02542100
O	-0.17402200	0.26853800	-0.99519700
O	-2.15982200	-1.15495600	-0.51798100
O	-0.06930800	-1.53161600	0.67712700
O	-1.35437900	0.46121600	1.16455500
H	-2.24299000	0.98208600	0.98043100
H	0.89522800	-1.23692200	0.64960800
C	4.27600000	0.39986300	-0.44798200
C	2.76324300	0.20138300	-0.51122000
O	4.93820400	-0.12503500	0.41142700
O	2.38764200	-0.73781600	0.47259300
O	2.22800200	1.46105500	-0.30725600
H	4.70931800	1.08247600	-1.19784300
H	2.45392500	-0.22118100	-1.47518600

H	3.06224400	-0.75099200	1.17249800
H	1.28297800	1.41348800	-0.53297900
O	-4.75970200	-0.19624800	-0.70060000
H	-3.96466700	-0.74714200	-0.81115300
H	-5.46348200	-0.76498000	-0.37379800
O	-3.50379600	1.63689000	0.70651800
H	-4.11660800	1.03595300	0.20675300
H	-3.47462000	2.48642000	0.25413700

(SA)(P4)(H<sub>2</sub>O)

S	1.80965200	-0.50971600	0.13823500
O	0.74782800	-1.41420200	-0.26432300
O	3.08663200	-1.02760800	0.57666400
O	1.27869800	0.42506900	1.28358900
O	2.03340700	0.47263100	-1.07673400
H	2.94834400	0.87964800	-0.99321500
H	0.30492200	0.65106000	1.11909300
O	4.50613500	1.11358600	-0.55396600
H	4.62941300	0.36088500	0.04550700
H	4.83243900	1.90242700	-0.10924700
C	-3.47610100	0.18513200	0.36845500
C	-1.99962000	-0.21590400	0.31029300
O	-4.27009600	-0.81872400	-0.16401400
O	-3.61468700	1.42233400	-0.29759000
O	-1.74377700	-0.48238300	-1.03180800
O	-1.21612800	0.86023300	0.79968400
H	-3.79094800	0.36320400	1.39826300
H	-1.77155300	-1.07287600	0.95088500
H	-3.48794500	1.26654300	-1.24460500
H	-1.56236800	1.67645800	0.40093300
H	-0.86431500	-0.89220100	-1.10308700
H	-3.80219700	-1.20253000	-0.92078700