

*Supplement of*

**Enhancing acid-base-water ternary aerosol nucleation with organic acid: a case of tartaric acid**

**Chunyu Wang et al.**

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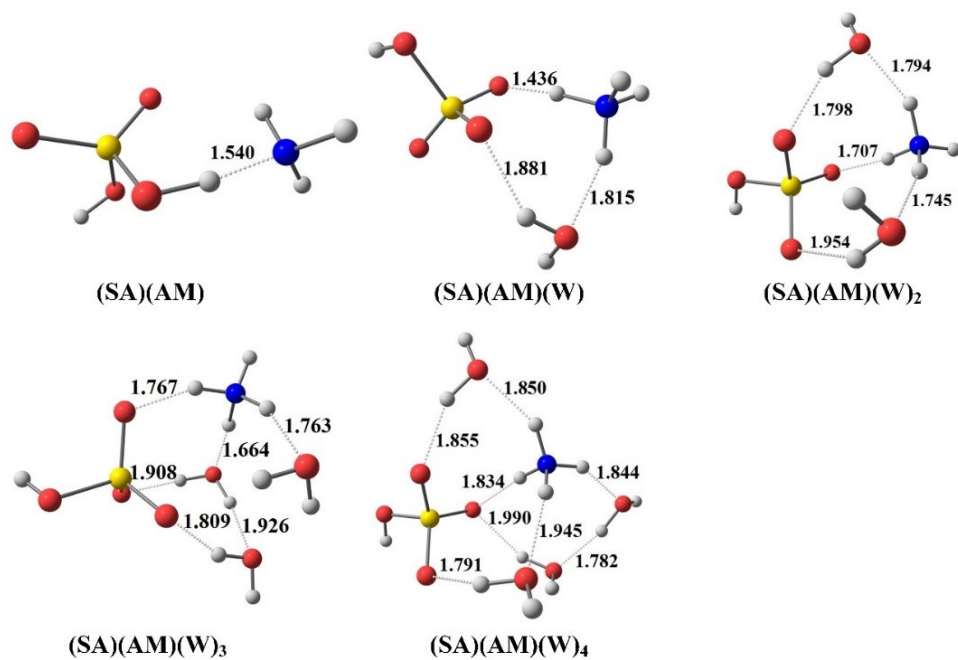


FIG. S1. Most stable configurations with hydrogen bonds and bond lengths ( $\text{\AA}$ ) of the hydrated (SA)(AM) clusters with 0-4 water molecules.

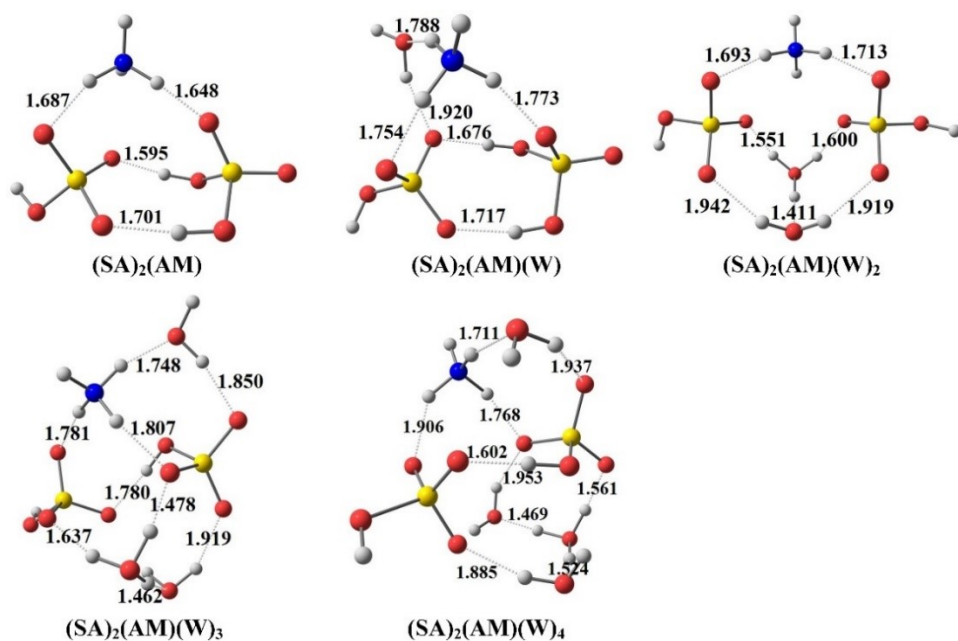


FIG. S2. Most stable configurations with hydrogen bonds and bond lengths ( $\text{\AA}$ ) of the hydrated (SA)<sub>2</sub>(AM) clusters with 0-4 water molecules.

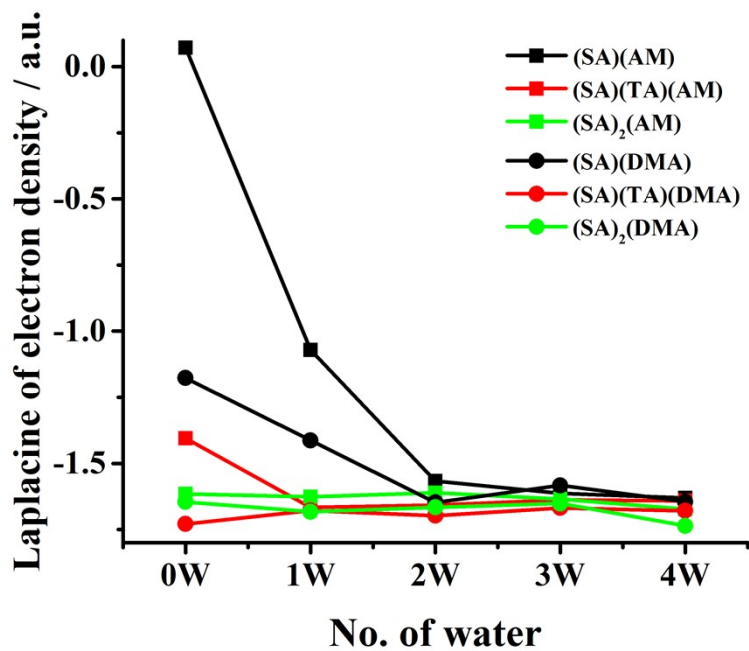


FIG. S3. Laplacian of electron densities at BCPs of the nitrogen-hydrogen bond in the clusters (a.u.).

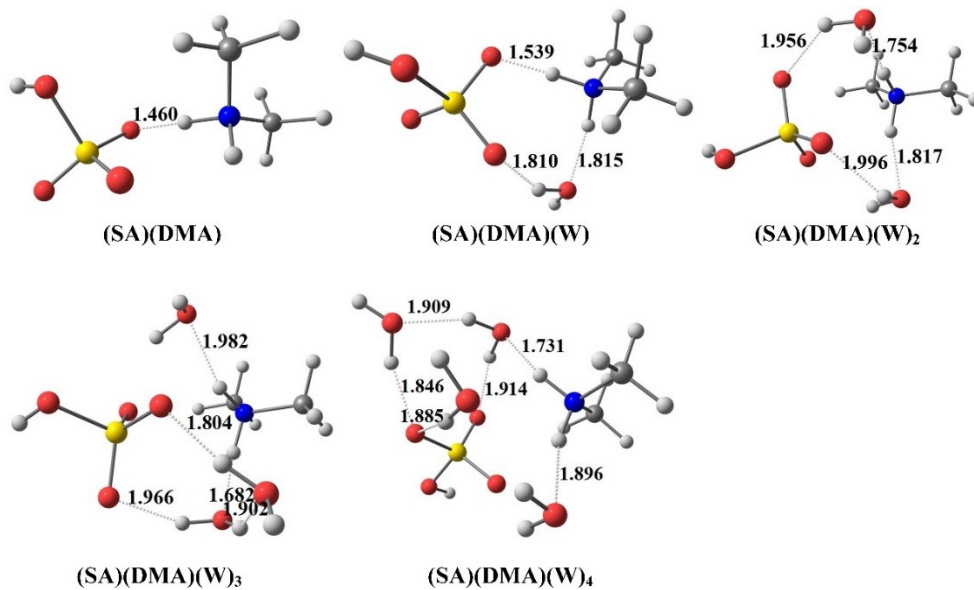
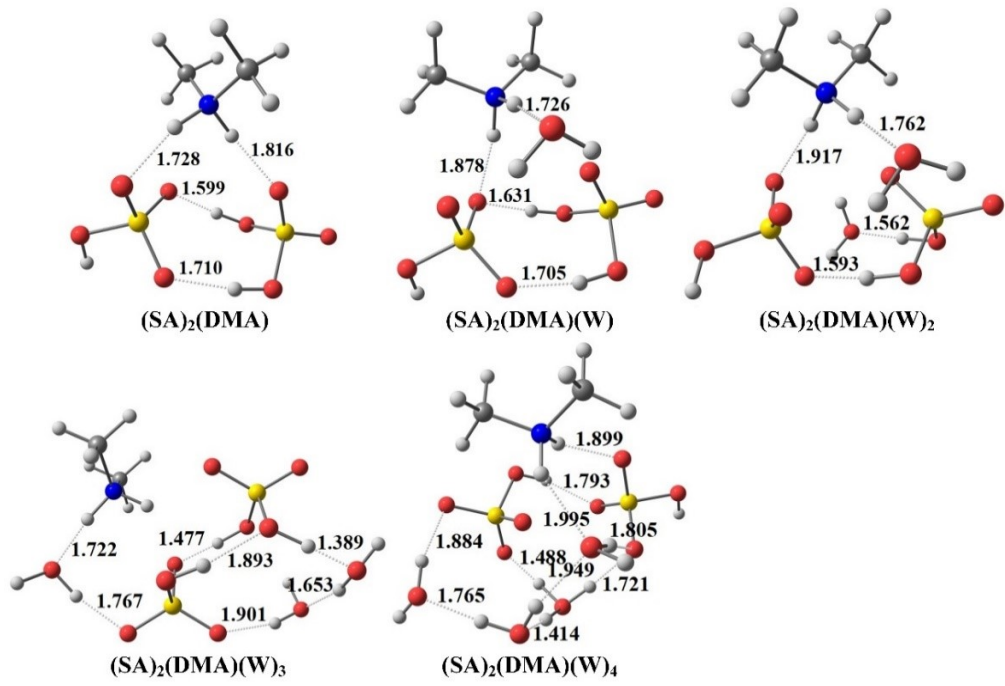
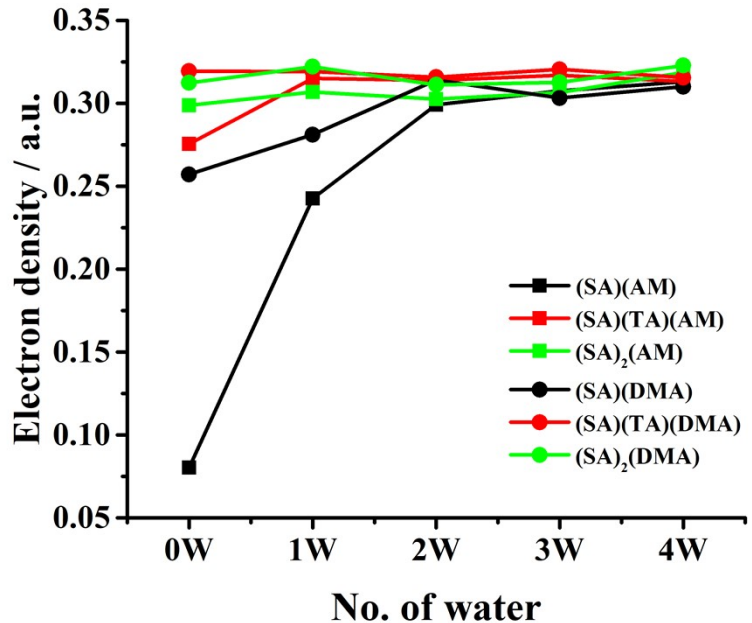


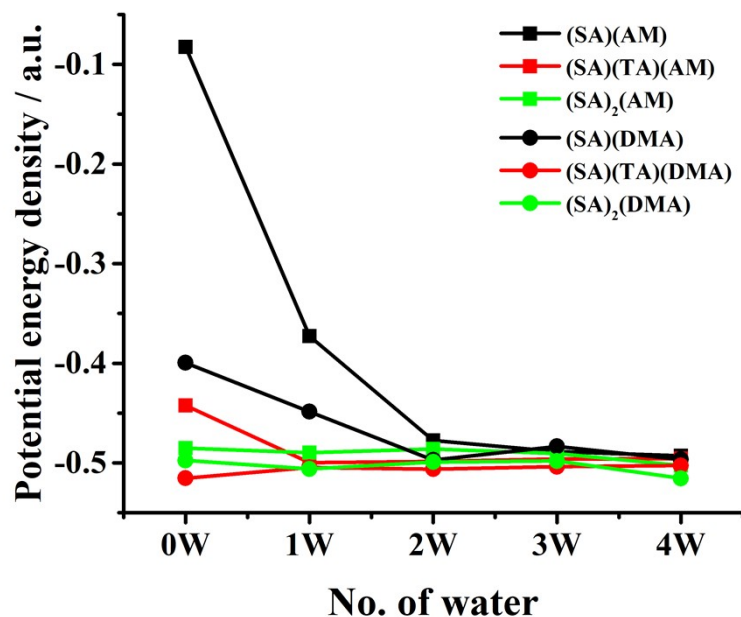
FIG. S4. Most stable configurations with hydrogen bonds and bond lengths (Å) of the hydrated (SA)(DMA) clusters with 0-4 water molecules.



**FIG. S5.** Most stable configurations with hydrogen bonds and bond lengths (Å) of the hydrated (SA)<sub>2</sub>(DMA) clusters with 0-4 water molecules.



**FIG. S6.** Electron densities at BCPs of the nitrogen-hydrogen bond in the clusters (a.u.).



**FIG. S7.** Potential energy densities at BCPs of the nitrogen-hydrogen bond in the clusters (a.u.).

**Table S1.** Laplacian bond order (LBO) of the newly formed covalent bond (nitrogen-hydrogen bond) between in the clusters (a.u.).

Clusters	Bonds	No. of water molecules				
		0	1	2	3	4
(SA)(AM)	N1-H1	-	0.338	0.542	0.575	0.592
(SA)(TA)(AM)	N1-H1	0.458	0.601	0.593	0.581	0.589
(SA) <sub>2</sub> (AM)	N1-H1	0.546	0.573	0.555	0.578	0.609
(SA)(DMA)	N2-H2	0.366	0.451	0.575	0.540	0.561
(SA)(TA)(DMA)	N2-H2	0.592	0.593	0.619	0.595	0.585
(SA) <sub>2</sub> (DMA)	N2-H2	0.566	0.600	0.605	0.578	0.607

Note: N1 and N2 are the nitrogen atoms on the AM molecule and DMA molecule, respectively; H1 and H2 are the hydrogen atoms on one of the hydroxyl functions of the SA molecule that bound to N1 and N2, respectively.

**Table S2.** Coordinates of optimized global free energy minima obtained at the M06-2X/6-311+G(2d,p) level of theory for monomers, (SA)(B)(W)<sub>n</sub>, (SA)(TA)(W)<sub>n</sub>, (SA)<sub>2</sub>(B)(W)<sub>n</sub> and (SA)(TA)(B)(W)<sub>n</sub> ( $n = 0-4$ ).

SA

S      0.000029000000      0.000121000000      -0.158793000000

O	0.665675000000	-1.063976000000	-0.821141000000
O	-0.664876000000	1.065610000000	-0.819645000000
O	-1.022927000000	-0.686827000000	0.840425000000
O	1.022185000000	0.685212000000	0.842506000000
H	-1.688675000000	-0.033684000000	1.101085000000
H	1.687748000000	0.031588000000	1.102437000000

### TA

O	0.164037000000	1.468084000000	0.793542000000
O	-0.164215000000	-1.468158000000	0.793178000000
O	2.256164000000	-0.659849000000	-1.167300000000
O	-2.256037000000	0.660299000000	-1.167053000000
O	2.610841000000	0.399912000000	0.775928000000
O	-2.610781000000	-0.400335000000	0.775691000000
C	0.468021000000	0.610280000000	-0.263993000000
C	-0.467975000000	-0.610191000000	-0.264220000000
C	1.896236000000	0.118978000000	-0.143558000000
C	-1.896204000000	-0.118986000000	-0.143720000000
H	0.357324000000	1.140218000000	-1.215308000000
H	-0.357266000000	-1.139932000000	-1.215646000000
H	0.871731000000	1.388898000000	1.448484000000
H	-0.872440000000	-1.389644000000	1.447612000000
H	3.158944000000	-0.967702000000	-1.002217000000
H	-3.158832000000	0.968059000000	-1.001874000000

### AM

N	0.000000000000	0.000000000000	0.112976000000
H	0.000000000000	0.941219000000	-0.263611000000
H	-0.815120000000	-0.470610000000	-0.263611000000
H	0.815120000000	-0.470610000000	-0.263611000000

### DMA

C	-0.026944000000	-0.224033000000	1.204850000000
N	-0.026944000000	0.589628000000	0.000000000000
C	-0.026944000000	-0.224033000000	-1.204850000000
H	0.029053000000	0.416428000000	2.085079000000
H	0.798251000000	-0.950916000000	1.244120000000
H	-0.964643000000	-0.781658000000	1.257343000000
H	0.786622000000	1.193300000000	0.000000000000
H	0.029053000000	0.416428000000	-2.085079000000
H	-0.964643000000	-0.781658000000	-1.257343000000
H	0.798251000000	-0.950916000000	-1.244120000000

### W

O	0.000000000000	0.000000000000	0.116481000000
H	0.000000000000	0.763464000000	-0.465925000000
H	0.000000000000	-0.763464000000	-0.465925000000

**(TA)(AM)**

O	-0.564212000000	-1.178859000000	1.128659000000
O	-0.635462000000	1.682931000000	0.472047000000
O	-2.839671000000	0.072200000000	-1.323241000000
O	1.804397000000	-0.474559000000	-0.975482000000
O	-3.129870000000	-0.488859000000	0.825937000000
O	1.925193000000	1.047317000000	0.668528000000
C	-0.929777000000	-0.638704000000	-0.106051000000
C	-0.180265000000	0.674824000000	-0.380950000000
C	-2.417518000000	-0.355484000000	-0.128226000000
C	1.304826000000	0.436189000000	-0.171952000000
H	-0.691826000000	-1.351892000000	-0.900413000000
H	-0.344399000000	0.961855000000	-1.424665000000
H	-1.272491000000	-0.976308000000	1.754877000000
H	0.092184000000	1.886186000000	1.077542000000
H	-3.782136000000	0.277497000000	-1.244288000000
H	2.781188000000	-0.613157000000	-0.739419000000
N	4.318534000000	-0.633768000000	-0.078945000000
H	4.593845000000	-1.480372000000	0.406979000000
H	5.103924000000	-0.334864000000	-0.646470000000
H	4.143386000000	0.085122000000	0.619957000000

**(TA)(DMA)**

O	1.113008000000	-1.492222000000	-0.444891000000
O	1.410419000000	1.359041000000	-1.140931000000
O	3.610354000000	0.541167000000	1.099711000000
O	-1.089464000000	0.221345000000	1.127894000000
O	3.728250000000	-0.947796000000	-0.569877000000
O	-1.184482000000	0.888393000000	-1.009231000000
C	1.588500000000	-0.485708000000	0.400033000000
C	0.933329000000	0.866461000000	0.076374000000
C	3.087755000000	-0.343118000000	0.242837000000
C	-0.571391000000	0.661233000000	0.012167000000
H	1.361722000000	-0.745339000000	1.437685000000
H	1.159290000000	1.570495000000	0.883771000000
H	1.790551000000	-1.650742000000	-1.116409000000
H	0.662103000000	1.345425000000	-1.755801000000
H	4.554848000000	0.616413000000	0.902572000000
H	-2.102281000000	-0.000027000000	0.980506000000
C	-4.274192000000	0.754459000000	0.095954000000
N	-3.556804000000	-0.413563000000	0.615697000000

C	-3.399861000000	-1.458182000000	-0.402986000000
H	-4.409521000000	1.485267000000	0.892626000000
H	-5.252796000000	0.485726000000	-0.315181000000
H	-3.666561000000	1.202853000000	-0.690137000000
H	-4.056986000000	-0.792397000000	1.413459000000
H	-2.882356000000	-2.313718000000	0.029725000000
H	-2.787514000000	-1.055621000000	-1.210166000000
H	-4.362381000000	-1.783701000000	-0.810214000000

**(SA)(TA)**

O	2.241924000000	1.611742000000	-0.120935000000
O	2.194938000000	-0.751900000000	1.568094000000
O	4.545224000000	-1.063301000000	-0.656774000000
O	-0.040895000000	-0.571563000000	-1.191062000000
O	4.807990000000	0.983712000000	0.219125000000
O	-0.318857000000	-0.067524000000	0.977743000000
C	2.637908000000	0.342286000000	-0.546098000000
C	1.842954000000	-0.728709000000	0.221015000000
C	4.115558000000	0.141014000000	-0.277077000000
C	0.369590000000	-0.426551000000	0.039592000000
H	2.458766000000	0.221503000000	-1.620163000000
H	2.052475000000	-1.708548000000	-0.213965000000
H	3.014490000000	2.045404000000	0.268529000000
H	1.648340000000	-0.104697000000	2.032301000000
H	5.484447000000	-1.131013000000	-0.431599000000
H	-1.000894000000	-0.348884000000	-1.271792000000
S	-3.537270000000	0.159653000000	-0.145026000000
O	-4.777519000000	0.838204000000	-0.253269000000
O	-2.663389000000	0.018952000000	-1.278502000000
O	-2.752178000000	0.764534000000	1.040836000000
O	-3.801182000000	-1.336698000000	0.317630000000
H	-1.791139000000	0.443229000000	1.023335000000
H	-4.554679000000	-1.348947000000	0.926087000000

**(SA)(W)**

S	0.578769000000	-0.068624000000	0.131227000000
O	-0.217148000000	0.364775000000	1.237408000000
O	1.756968000000	-0.846471000000	0.293285000000
O	-0.335934000000	-0.803571000000	-0.896046000000
O	0.967059000000	1.267019000000	-0.637732000000
H	-1.284378000000	-0.520738000000	-0.744751000000
H	1.716588000000	1.079572000000	-1.220927000000
O	-2.670846000000	0.094683000000	-0.117309000000
H	-2.295053000000	0.417331000000	0.714598000000



H	-3.398252000000	-0.489653000000	0.114596000000
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**(SA)(AM)**

S	0.601066000000	-0.113814000000	-0.090640000000
O	-0.103170000000	-0.091658000000	-1.335803000000
O	1.779915000000	-0.890299000000	0.100650000000
O	0.983856000000	1.413447000000	0.183683000000
O	-0.389861000000	-0.428342000000	1.051868000000
H	1.715656000000	1.429298000000	0.815846000000
H	-1.370170000000	-0.231574000000	0.727923000000
N	-2.727527000000	0.040962000000	0.053754000000
H	-2.448948000000	0.084766000000	-0.924271000000
H	-3.418227000000	-0.694881000000	0.155077000000
H	-3.168606000000	0.921503000000	0.296201000000

**(SA)(DMA)**

S	-1.270827000000	-0.175350000000	0.059219000000
O	-0.574293000000	0.060312000000	1.311436000000
O	-2.501363000000	-0.908588000000	0.083311000000
O	-1.646239000000	1.326500000000	-0.421594000000
O	-0.315071000000	-0.657424000000	-0.976980000000
H	-2.400183000000	1.253070000000	-1.020699000000
H	1.015904000000	-0.428880000000	-0.422397000000
C	3.101826000000	-0.893366000000	-0.140133000000
N	1.893046000000	-0.115490000000	0.173602000000
C	2.036484000000	1.343056000000	-0.016366000000
H	2.897708000000	-1.949372000000	0.020683000000
H	3.928784000000	-0.573620000000	0.492727000000
H	3.359011000000	-0.729990000000	-1.184994000000
H	1.555128000000	-0.288073000000	1.123661000000
H	1.087641000000	1.808767000000	0.243133000000
H	2.267866000000	1.533239000000	-1.062749000000
H	2.835926000000	1.724345000000	0.617525000000

**(SA)(AM)(W)<sub>1</sub>**

S	-0.843138000000	-0.097706000000	-0.046949000000
O	-1.289221000000	-1.246010000000	-0.785053000000
O	0.098893000000	-0.333523000000	1.041347000000
O	-0.351513000000	1.008554000000	-0.907568000000
O	-2.134487000000	0.500680000000	0.693650000000
H	0.975948000000	1.344228000000	-0.473497000000
H	-2.909179000000	0.213808000000	0.192812000000
N	1.996765000000	1.432470000000	-0.026911000000
H	2.558518000000	2.168323000000	-0.442461000000

H	2.439339000000	0.501178000000	-0.133353000000
H	1.867777000000	1.597888000000	0.969364000000
O	2.487133000000	-1.301174000000	0.074216000000
H	1.599763000000	-1.317207000000	0.478213000000
H	2.494255000000	-2.000418000000	-0.584256000000

**(SA)(AM)(W)<sub>2</sub>**

S	-1.010219000000	-0.102052000000	0.053407000000
O	-0.098591000000	-0.456509000000	-1.029434000000
O	-1.464197000000	1.277103000000	0.019606000000
O	-2.295245000000	-1.011998000000	-0.232493000000
O	-0.505483000000	-0.511090000000	1.368014000000
H	-3.027345000000	-0.662949000000	0.293400000000
H	1.104189000000	0.049823000000	1.457806000000
N	2.038163000000	0.377418000000	1.106241000000
H	2.427037000000	-0.418613000000	0.566237000000
H	1.837780000000	1.170490000000	0.449821000000
H	2.654143000000	0.663837000000	1.860030000000
O	2.272545000000	-1.733527000000	-0.644326000000
H	2.316166000000	-2.688796000000	-0.562533000000
H	1.351695000000	-1.510625000000	-0.887308000000
O	1.093869000000	2.240023000000	-0.711409000000
H	1.048141000000	1.694020000000	-1.506792000000
H	0.161362000000	2.261707000000	-0.428522000000

**(SA)(AM)(W)<sub>3</sub>**

S	1.285153000000	-0.015559000000	-0.040244000000
O	1.173585000000	-0.412845000000	1.352906000000
O	0.423755000000	-0.775356000000	-0.944788000000
O	1.194745000000	1.429629000000	-0.241952000000
O	2.748834000000	-0.440020000000	-0.525172000000
H	-0.447634000000	2.041763000000	-0.034432000000
H	3.392359000000	-0.005604000000	0.050789000000
N	-1.475587000000	1.981037000000	0.121265000000
H	-1.604249000000	1.351632000000	0.961478000000
H	-1.897370000000	2.894365000000	0.252548000000
H	-1.876107000000	1.472614000000	-0.697721000000
O	-1.821310000000	-1.951705000000	0.075907000000
H	-0.903426000000	-1.763239000000	-0.206372000000
H	-1.887282000000	-2.903182000000	0.191270000000
O	-1.514159000000	0.072903000000	2.025090000000
H	-0.555144000000	-0.088817000000	2.089608000000
H	-1.838201000000	-0.714322000000	1.555649000000
O	-2.084089000000	0.172364000000	-1.865502000000

H	-1.147412000000	-0.060721000000	-1.973632000000
H	-2.439744000000	-0.602564000000	-1.406053000000

**(SA)(AM)(W)<sub>4</sub>**

S	-1.457045000000	-0.417530000000	-0.187414000000
O	-1.314205000000	-1.525648000000	0.747954000000
O	-1.591339000000	0.884719000000	0.433032000000
O	-0.427454000000	-0.447290000000	-1.235980000000
O	-2.858281000000	-0.632477000000	-0.926729000000
H	0.828643000000	0.731018000000	-0.604311000000
H	-2.905565000000	-1.552115000000	-1.221333000000
N	1.421787000000	1.258788000000	0.062238000000
H	2.401751000000	1.200954000000	-0.251917000000
H	1.321059000000	0.774711000000	0.966995000000
H	1.048376000000	2.217545000000	0.122784000000
O	1.961330000000	-1.808660000000	-0.381638000000
H	1.100038000000	-1.644968000000	-0.798365000000
H	1.777066000000	-1.798222000000	0.568350000000
O	0.925530000000	-0.760158000000	2.094035000000
H	0.030670000000	-1.069455000000	1.838683000000
H	0.971600000000	-0.794746000000	3.052805000000
O	3.813979000000	0.140479000000	-0.780838000000
H	4.474241000000	0.055063000000	-1.471065000000
H	3.296874000000	-0.691336000000	-0.758619000000
O	-0.402641000000	3.362922000000	0.201952000000
H	-1.065773000000	2.650860000000	0.222375000000
H	-0.774110000000	4.078569000000	-0.317737000000

**(SA)(DMA)(W)<sub>1</sub>**

S	1.453582000000	-0.060411000000	-0.120417000000
O	0.702796000000	0.832254000000	0.758988000000
O	2.433410000000	0.541833000000	-0.980840000000
O	2.271292000000	-0.976969000000	0.922199000000
O	0.536960000000	-0.992731000000	-0.809436000000
H	3.101399000000	-1.218986000000	0.492543000000
H	-0.902979000000	-0.627209000000	-0.409183000000
C	-2.892123000000	-0.999949000000	-0.952736000000
N	-1.890976000000	-0.331353000000	-0.102802000000
C	-2.036383000000	-0.626698000000	1.338872000000
H	-2.703259000000	-0.742946000000	-1.992537000000
H	-3.892731000000	-0.681252000000	-0.665029000000
H	-2.798057000000	-2.076814000000	-0.824480000000
H	-1.915315000000	0.693955000000	-0.233205000000
H	-1.247822000000	-0.098333000000	1.869014000000

H	-1.926135000000	-1.699731000000	1.486447000000
H	-3.017584000000	-0.300264000000	1.679914000000
O	-1.370514000000	2.408203000000	0.010825000000
H	-0.472085000000	2.115082000000	0.259666000000
H	-1.266429000000	3.181709000000	-0.547557000000

**(SA)(DMA)(W)<sub>2</sub>**

S	-1.400243000000	-0.001796000000	0.112885000000
O	-0.995262000000	1.111949000000	0.958795000000
O	-1.113794000000	-1.298266000000	0.720146000000
O	-2.994071000000	0.084697000000	-0.045912000000
O	-0.933252000000	0.112277000000	-1.266358000000
H	-3.384625000000	-0.021572000000	0.832017000000
H	1.303325000000	0.844146000000	-0.003720000000
C	3.187385000000	0.105834000000	-0.328881000000
N	1.828835000000	-0.020890000000	0.239315000000
C	1.810488000000	-0.249753000000	1.702261000000
H	3.101252000000	0.297692000000	-1.395657000000
H	3.730031000000	-0.821835000000	-0.158702000000
H	3.697992000000	0.937594000000	0.152177000000
H	1.351400000000	-0.816260000000	-0.244724000000
H	0.774769000000	-0.325434000000	2.022686000000
H	2.301796000000	0.587674000000	2.194331000000
H	2.345714000000	-1.173526000000	1.915717000000
O	0.761503000000	2.335925000000	-0.889174000000
H	0.131963000000	1.795688000000	-1.396358000000
H	0.201644000000	2.654335000000	-0.168568000000
O	0.743749000000	-2.205459000000	-1.127220000000
H	0.042521000000	-2.338492000000	-0.465612000000
H	0.266036000000	-1.710495000000	-1.807438000000

**(SA)(DMA)(W)<sub>3</sub>**

S	1.526646000000	-0.092678000000	-0.141802000000
O	0.804938000000	0.144213000000	1.111191000000
O	1.839173000000	1.101533000000	-0.901965000000
O	2.928443000000	-0.676452000000	0.384412000000
O	0.905567000000	-1.151548000000	-0.932674000000
H	3.528232000000	-0.729137000000	-0.371980000000
H	-1.103691000000	-0.758652000000	0.338668000000
C	-2.296417000000	-1.326944000000	-1.213647000000
N	-1.843591000000	-0.322901000000	-0.229925000000
C	-2.909118000000	0.163776000000	0.670536000000
H	-1.438591000000	-1.615150000000	-1.816837000000
H	-3.071055000000	-0.886486000000	-1.838522000000

H	-2.682027000000	-2.191092000000	-0.675918000000
H	-1.413963000000	0.500092000000	-0.725474000000
H	-2.484763000000	0.921996000000	1.326519000000
H	-3.289587000000	-0.676353000000	1.249086000000
H	-3.707144000000	0.597183000000	0.070222000000
O	-0.536105000000	-2.489921000000	1.120106000000
H	0.104738000000	-2.435446000000	0.392690000000
H	-0.059928000000	-2.088480000000	1.856120000000
O	-0.594918000000	2.488409000000	1.354621000000
H	-0.215592000000	3.220219000000	1.847044000000
H	0.061008000000	1.764455000000	1.384064000000
O	-0.826703000000	1.942612000000	-1.361105000000
H	-0.788182000000	2.460164000000	-0.537718000000
H	0.109399000000	1.768080000000	-1.557668000000

**(SA)(DMA)(W)<sub>4</sub>**

S	-1.563140000000	-0.655395000000	-0.068939000000
O	-1.719056000000	0.553573000000	0.736256000000
O	-0.519753000000	-1.539617000000	0.433538000000
O	-2.962310000000	-1.399292000000	0.170676000000
O	-1.465614000000	-0.423819000000	-1.503278000000
H	-3.011233000000	-2.145866000000	-0.441115000000
H	-0.334981000000	1.079791000000	-1.855462000000
C	1.866503000000	-1.294052000000	-1.633335000000
N	1.962978000000	-0.322983000000	-0.524167000000
C	3.330339000000	0.161141000000	-0.257385000000
H	0.818368000000	-1.554679000000	-1.762018000000
H	2.449891000000	-2.178239000000	-1.382751000000
H	2.254710000000	-0.829711000000	-2.538301000000
H	1.605744000000	-0.748111000000	0.346698000000
H	3.281791000000	0.857385000000	0.576367000000
H	3.710933000000	0.659663000000	-1.146982000000
H	3.961382000000	-0.686352000000	0.003098000000
O	0.436554000000	1.642787000000	-1.670252000000
H	0.089612000000	2.351915000000	-1.104321000000
H	1.353003000000	0.493310000000	-0.755505000000
O	1.738888000000	-1.370084000000	2.132291000000
H	1.596205000000	-0.475438000000	2.472169000000
H	0.846227000000	-1.724524000000	2.017002000000
O	0.871188000000	1.268125000000	1.635167000000
H	-0.026924000000	0.924211000000	1.480401000000
H	0.743867000000	2.223144000000	1.591957000000
O	-0.913832000000	3.149120000000	0.310505000000
H	-1.511397000000	3.896651000000	0.232107000000
H	-1.467374000000	2.355187000000	0.423938000000

**(SA)(TA)(W)<sub>1</sub>**

O	2.322504000000	-1.522447000000	1.055019000000
O	1.833421000000	1.310652000000	0.366283000000
O	-0.022242000000	-0.491189000000	-1.419462000000
O	4.672565000000	-0.484939000000	-0.816897000000
O	-0.284980000000	-1.247580000000	0.675375000000
O	4.420475000000	1.060062000000	0.791093000000
C	1.921387000000	-1.040783000000	-0.189405000000
C	2.495949000000	0.362508000000	-0.432307000000
C	0.410243000000	-0.945352000000	-0.275021000000
C	3.968366000000	0.364233000000	-0.072840000000
H	2.273768000000	-1.705755000000	-0.984794000000
H	2.383038000000	0.623155000000	-1.488105000000
H	1.539470000000	-1.584949000000	1.619486000000
H	2.461080000000	1.623006000000	1.037141000000
H	-1.015577000000	-0.341582000000	-1.384231000000
H	5.591369000000	-0.465681000000	-0.510905000000
S	-3.344213000000	-0.016239000000	-0.029048000000
O	-2.536482000000	0.114791000000	-1.236441000000
O	-4.752015000000	0.040587000000	-0.140700000000
O	-2.986019000000	-1.374190000000	0.655257000000
O	-2.833377000000	1.039099000000	0.981759000000
H	-2.004514000000	-1.433244000000	0.747443000000
H	-1.995004000000	1.500465000000	0.634013000000
O	-0.797193000000	2.229906000000	0.011600000000
H	0.118363000000	1.940246000000	0.172916000000
H	-0.913518000000	2.262485000000	-0.943850000000

**(SA)(TA)(W)<sub>2</sub>**

O	1.895581000000	0.837057000000	1.004283000000
O	2.554091000000	-1.934349000000	0.232994000000
O	4.764139000000	0.040059000000	-0.952222000000
O	0.074962000000	-0.003400000000	-1.438635000000
O	4.513914000000	0.594708000000	1.207496000000
O	-0.079015000000	-1.660920000000	0.065044000000
C	2.568369000000	0.443326000000	-0.164833000000
C	2.082645000000	-0.940619000000	-0.622336000000
C	4.054187000000	0.374300000000	0.123247000000
C	0.566931000000	-0.911918000000	-0.641719000000
H	2.387156000000	1.172465000000	-0.959114000000
H	2.443372000000	-1.118103000000	-1.640422000000
H	2.536496000000	0.832162000000	1.732172000000
H	1.802201000000	-2.276175000000	0.736220000000
H	5.694184000000	-0.028210000000	-0.690890000000
H	-0.916824000000	0.059555000000	-1.326882000000

S	-3.189961000000	-0.397968000000	0.121596000000
O	-2.490871000000	0.284955000000	-0.974725000000
O	-4.604524000000	-0.347057000000	0.122400000000
O	-2.775147000000	-1.902754000000	0.072471000000
O	-2.600667000000	0.102748000000	1.440126000000
H	-1.789219000000	-1.955295000000	0.095336000000
H	-1.776134000000	0.774791000000	1.321108000000
O	-1.688839000000	2.948279000000	-1.043510000000
H	-2.304248000000	2.226428000000	-1.240496000000
H	-2.188454000000	3.766958000000	-1.097145000000
O	-0.772601000000	1.716553000000	1.189357000000
H	-0.963333000000	2.292146000000	0.418937000000
H	0.153202000000	1.423195000000	1.138861000000

**(SA)(TA)(W)<sub>3</sub>**

O	1.083870000000	-0.721972000000	1.489545000000
O	1.559938000000	0.413873000000	-1.241529000000
O	0.130144000000	-2.257385000000	-1.551491000000
O	4.220029000000	-1.149552000000	0.463659000000
O	-0.882388000000	-2.323867000000	0.438136000000
O	3.636181000000	1.001979000000	0.262332000000
C	1.360856000000	-1.469605000000	0.343989000000
C	2.201765000000	-0.690926000000	-0.682009000000
C	0.074374000000	-2.053869000000	-0.241674000000
C	3.417777000000	-0.156088000000	0.055059000000
H	1.962738000000	-2.328459000000	0.659549000000
H	2.545810000000	-1.390795000000	-1.451859000000
H	0.611184000000	0.099130000000	1.242657000000
H	0.601900000000	0.258755000000	-1.346933000000
H	-0.776617000000	-2.460350000000	-1.860751000000
H	4.947409000000	-0.750965000000	0.962338000000
S	-1.430782000000	1.506894000000	-0.050774000000
O	-1.125933000000	0.352061000000	-0.936669000000
O	-2.861637000000	1.609444000000	0.181005000000
O	-0.617861000000	1.436789000000	1.168810000000
O	-1.004332000000	2.796003000000	-0.802794000000
H	-1.387071000000	0.201736000000	2.556938000000
H	-0.004137000000	2.955779000000	-0.654023000000
N	-3.408774000000	-1.054201000000	0.747353000000
H	-3.007143000000	-1.629563000000	-0.001795000000
H	-4.326460000000	-1.399323000000	1.011308000000
H	-3.459217000000	-0.068712000000	0.419700000000
O	-1.637754000000	-0.719223000000	2.738445000000
H	-0.863329000000	-1.218010000000	2.431510000000
H	-2.742773000000	-1.045440000000	1.578290000000
O	-2.522899000000	-1.637487000000	-2.050197000000

H	-2.134522000000	-0.756705000000	-1.862309000000
H	-3.016194000000	-1.558231000000	-2.870882000000
O	1.506309000000	3.090631000000	-0.408429000000
H	1.908237000000	2.226554000000	-0.617225000000
H	1.696157000000	3.226281000000	0.525597000000

**(SA)(TA)(W)<sub>4</sub>**

O	-2.208511000000	-0.829051000000	1.057011000000
O	-3.395725000000	1.699294000000	0.083056000000
O	-5.117115000000	-0.740018000000	-0.998065000000
O	-0.486216000000	0.177235000000	-1.276438000000
O	-4.827766000000	-1.086412000000	1.199389000000
O	-0.779102000000	2.069261000000	-0.101161000000
C	-2.909474000000	-0.641002000000	-0.147952000000
C	-2.688078000000	0.776946000000	-0.687465000000
C	-4.387560000000	-0.850992000000	0.109873000000
C	-1.198165000000	1.079785000000	-0.660395000000
H	-2.566789000000	-1.366903000000	-0.889647000000
H	-3.023687000000	0.807879000000	-1.730444000000
H	-2.861482000000	-0.889068000000	1.771807000000
H	-2.755876000000	2.330228000000	0.442222000000
H	-6.049303000000	-0.841820000000	-0.756482000000
H	0.511621000000	0.333258000000	-1.215723000000
S	2.897517000000	0.459658000000	-0.038421000000
O	4.080142000000	-0.367928000000	0.049806000000
O	2.061624000000	0.065062000000	-1.218438000000
O	2.067268000000	0.503105000000	1.167849000000
O	3.391316000000	1.905449000000	-0.311436000000
H	0.942847000000	-0.836261000000	1.374322000000
H	2.704865000000	2.559301000000	0.054615000000
O	1.584455000000	-2.480696000000	-0.776096000000
H	1.808641000000	-1.593499000000	-1.178999000000
H	2.479244000000	-2.858628000000	-0.454975000000
O	1.572696000000	3.344742000000	0.792280000000
H	0.742217000000	3.022565000000	0.401270000000
H	1.612811000000	2.892117000000	1.643841000000
O	0.437357000000	-1.666933000000	1.223303000000
H	-0.505895000000	-1.425098000000	1.161674000000
H	1.009279000000	-2.198413000000	0.096563000000
O	3.917945000000	-3.072428000000	0.015560000000
H	4.105748000000	-3.506995000000	0.851938000000
H	4.198192000000	-2.137079000000	0.105435000000

**(SA)<sub>2</sub>(AM)**

S	1.777048000000	-0.362988000000	-0.052525000000
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O	2.406331000000	0.721953000000	-0.804456000000
O	1.080505000000	0.182655000000	1.128180000000
O	2.964558000000	-1.271358000000	0.485973000000
O	0.973771000000	-1.287829000000	-0.817015000000
H	1.458380000000	2.071523000000	-0.449717000000
H	3.676475000000	-0.699365000000	0.803116000000
S	-2.086578000000	-0.103346000000	-0.009251000000
O	-1.432703000000	-0.421419000000	1.366331000000
O	-3.492041000000	-0.098731000000	0.144200000000
O	-1.703703000000	-1.315726000000	-0.906722000000
O	-1.430849000000	1.075120000000	-0.553923000000
H	-0.440250000000	-0.256094000000	1.328932000000
H	-0.716762000000	-1.362787000000	-0.991532000000
N	0.682760000000	2.658349000000	-0.046537000000
H	-0.198569000000	2.103635000000	-0.181206000000
H	0.614610000000	3.570450000000	-0.489513000000
H	0.852326000000	2.748204000000	0.953560000000

**(SA)<sub>2</sub>(AM)(W)<sub>1</sub>**

S	2.251136000000	0.142665000000	-0.050056000000
O	2.259449000000	-1.372837000000	0.314981000000
O	1.403363000000	0.823970000000	0.907117000000
O	1.535625000000	0.192522000000	-1.438046000000
O	3.593483000000	0.552412000000	-0.225699000000
H	1.324181000000	-1.685697000000	0.406083000000
H	0.550654000000	0.136795000000	-1.309292000000
S	-1.418155000000	-0.971470000000	0.091294000000
O	-0.366339000000	-1.954102000000	0.274399000000
O	-2.589318000000	-1.713473000000	-0.698360000000
O	-1.058155000000	0.110480000000	-0.839810000000
O	-1.997536000000	-0.465842000000	1.325364000000
H	-2.796131000000	-2.538368000000	-0.236786000000
N	-0.997953000000	2.098915000000	1.340924000000
H	-0.032158000000	1.853983000000	1.058483000000
H	-1.505156000000	2.528387000000	0.546168000000
H	-1.463847000000	1.189912000000	1.549114000000
O	-2.302510000000	2.567280000000	-1.053366000000
H	-2.111683000000	1.648104000000	-1.301690000000
H	-3.145496000000	2.804994000000	-1.445404000000
H	-0.986869000000	2.707086000000	2.154397000000

**(SA)<sub>2</sub>(AM)(W)<sub>2</sub>**

S	2.445584000000	0.170349000000	-0.141069000000
O	2.338043000000	-1.139984000000	-0.749358000000

O	3.985545000000	0.367265000000	0.224509000000
O	2.156317000000	1.311604000000	-0.990075000000
H	4.343338000000	-0.488242000000	0.498197000000
S	-2.444498000000	0.155146000000	-0.128213000000
O	-2.262419000000	-1.102303000000	-0.823875000000
O	-1.700782000000	0.253292000000	1.136922000000
O	-3.960822000000	0.182564000000	0.372112000000
O	-2.254472000000	1.338887000000	-0.957658000000
H	-0.894066000000	2.190566000000	-0.359668000000
O	1.707776000000	0.254063000000	1.138519000000
O	0.022973000000	-1.623226000000	1.503103000000
N	-0.028986000000	2.445917000000	0.171431000000
O	0.018851000000	-2.693177000000	-0.723781000000
H	-0.050797000000	1.895798000000	1.034289000000
H	0.826468000000	2.144129000000	-0.354125000000
H	-4.532083000000	-0.021698000000	-0.381486000000
H	0.806512000000	-2.277321000000	-1.113591000000
H	-0.759515000000	-2.259910000000	-1.115089000000
H	0.793814000000	-0.964393000000	1.430197000000
H	0.020751000000	-2.167366000000	0.585715000000
H	-0.776139000000	-1.012227000000	1.459804000000
H	-0.000837000000	3.439442000000	0.380924000000

**(SA)<sub>2</sub>(AM)(W)<sub>3</sub>**

S	2.076518000000	-0.793624000000	-0.183756000000
O	3.619389000000	-0.914115000000	-0.558006000000
O	1.462654000000	-2.067270000000	-0.524917000000
O	2.102699000000	-0.502867000000	1.243997000000
O	1.539797000000	0.315764000000	-0.980992000000
H	3.691456000000	-1.253364000000	-1.461361000000
S	-1.793755000000	0.839729000000	-0.157926000000
O	-1.138146000000	-0.242190000000	-1.126713000000
O	-3.195776000000	0.515003000000	-0.201105000000
O	-1.193643000000	0.531146000000	1.184154000000
O	-1.392558000000	2.152048000000	-0.608492000000
H	-0.184694000000	-0.027379000000	-1.255156000000
N	-0.887080000000	-2.250118000000	0.979259000000
H	-1.779975000000	-2.464810000000	0.485582000000
H	-0.756386000000	-2.855660000000	1.784557000000
H	-0.071150000000	-2.326535000000	0.341637000000
H	-0.951229000000	-1.257066000000	1.277315000000
O	0.916823000000	1.775151000000	1.698391000000
H	1.522737000000	0.983412000000	1.611941000000
H	1.095358000000	2.388235000000	0.867475000000
H	-0.016054000000	1.351260000000	1.538503000000

H	-3.442249000000	-1.309270000000	-0.389545000000
O	-3.341873000000	-2.273862000000	-0.274824000000
H	-4.209212000000	-2.610495000000	-0.038197000000
H	1.645556000000	2.386218000000	-0.946532000000
O	1.226372000000	3.079788000000	-0.414458000000
H	0.295276000000	3.059833000000	-0.700397000000

**(SA)<sub>2</sub>(AM)(W)<sub>4</sub>**

S	-1.875855000000	0.632381000000	0.047334000000
O	-0.909952000000	0.315872000000	1.117383000000
O	-2.992128000000	-0.305901000000	0.012483000000
O	-1.086225000000	0.338441000000	-1.312015000000
O	-2.240063000000	2.030492000000	0.025062000000
H	-0.107394000000	0.485596000000	-1.158491000000
O	-0.125080000000	-2.239435000000	1.935298000000
H	0.679124000000	-2.273458000000	1.390074000000
H	-1.253365000000	-2.546616000000	1.045908000000
H	-0.272023000000	-1.283979000000	2.037166000000
O	-2.008468000000	-2.650999000000	0.329708000000
H	-1.516985000000	-2.696754000000	-0.571992000000
H	-2.505440000000	-1.763816000000	0.285547000000
O	0.004169000000	3.396418000000	-0.997614000000
H	0.408022000000	2.886987000000	-1.708386000000
H	0.644923000000	2.886924000000	0.504519000000
H	-0.911666000000	3.073730000000	-0.923580000000
S	2.108761000000	-0.323939000000	-0.095907000000
O	1.460372000000	0.711410000000	-0.917626000000
O	1.531136000000	-1.647997000000	-0.314585000000
O	2.254193000000	0.052808000000	1.292053000000
O	3.614643000000	-0.401753000000	-0.618645000000
H	3.616340000000	-0.766849000000	-1.514036000000
N	0.783513000000	2.437195000000	1.443246000000
H	-0.005265000000	1.768638000000	1.559698000000
H	1.627424000000	1.846550000000	1.443617000000
H	-1.039350000000	-1.602854000000	-2.130417000000
O	-0.698831000000	-2.460776000000	-1.836193000000
H	0.188196000000	-2.248045000000	-1.492817000000
H	0.806253000000	3.129883000000	2.185174000000

**(SA)<sub>2</sub>(DMA)**

S	1.324549000000	-1.305294000000	-0.122029000000
O	0.238653000000	-2.010848000000	-0.783416000000
O	2.143236000000	-0.450502000000	-0.960276000000
O	0.872598000000	-0.602175000000	1.093811000000

O	2.342971000000	-2.431843000000	0.358525000000
H	-0.708615000000	-0.583532000000	1.329652000000
H	1.832681000000	-3.187505000000	0.681266000000
S	-2.235499000000	0.138861000000	0.047495000000
O	-1.708185000000	-0.476703000000	1.378379000000
O	-3.567100000000	0.576279000000	0.244246000000
O	-1.236599000000	1.076012000000	-0.430427000000
O	-2.272325000000	-1.069419000000	-0.938182000000
H	0.373553000000	1.631015000000	0.200688000000
H	-1.359306000000	-1.447803000000	-1.018207000000
C	1.125844000000	3.067718000000	-1.051539000000
N	1.306589000000	1.996378000000	-0.049001000000
C	2.055194000000	2.397494000000	1.160506000000
H	0.535395000000	2.668471000000	-1.872459000000
H	2.101433000000	3.394069000000	-1.405614000000
H	0.597261000000	3.899002000000	-0.589450000000
H	1.767446000000	1.167056000000	-0.481845000000
H	2.121318000000	1.532656000000	1.815981000000
H	1.526048000000	3.210299000000	1.654075000000
H	3.049629000000	2.726869000000	0.866370000000

**(SA)<sub>2</sub>(DMA)(W)<sub>1</sub>**

S	2.260880000000	0.271195000000	-0.057615000000
O	1.861995000000	-0.316888000000	-1.447383000000
O	3.496548000000	0.949368000000	-0.191266000000
O	1.101672000000	0.969874000000	0.461093000000
O	2.505429000000	-0.990607000000	0.828098000000
H	-1.293182000000	1.733441000000	0.706481000000
H	1.662028000000	-1.510289000000	0.864972000000
S	-1.052247000000	-1.553294000000	-0.027980000000
O	-1.903548000000	-0.809263000000	0.870079000000
O	0.124634000000	-2.179437000000	0.555598000000
O	-1.981794000000	-2.749962000000	-0.520807000000
O	-0.714924000000	-0.780704000000	-1.246553000000
H	-1.425835000000	-3.415867000000	-0.948710000000
H	0.888838000000	-0.555288000000	-1.440520000000
C	-2.958902000000	1.814645000000	-0.531975000000
N	-1.495344000000	1.836576000000	-0.317501000000
C	-0.831065000000	3.051787000000	-0.836189000000
H	-3.345853000000	0.881899000000	-0.129827000000
H	-3.162025000000	1.879282000000	-1.599289000000
H	-3.402461000000	2.664786000000	-0.017302000000
H	-1.083641000000	0.990265000000	-0.742930000000
H	0.232499000000	2.975676000000	-0.627102000000
H	-1.254146000000	3.921145000000	-0.336593000000
H	-1.003786000000	3.122676000000	-1.908478000000

O	-0.949023000000	1.403769000000	2.365450000000
H	-1.279424000000	0.493701000000	2.320956000000
H	0.008149000000	1.308345000000	2.264868000000

**(SA)<sub>2</sub>(DMA)(W)<sub>2</sub>**

S	-2.097595000000	0.318191000000	-0.155085000000
O	-3.047569000000	-0.635148000000	0.610792000000
O	-2.837186000000	1.418638000000	-0.676923000000
O	-0.956620000000	0.578482000000	0.694039000000
O	-1.618586000000	-0.509739000000	-1.389157000000
H	1.362306000000	0.935281000000	0.961872000000
H	-0.939765000000	-1.200120000000	-1.104560000000
S	1.376788000000	-1.376535000000	-0.240614000000
O	1.527045000000	-0.305432000000	-1.210978000000
O	1.534812000000	-0.965188000000	1.142077000000
O	0.161785000000	-2.175633000000	-0.494226000000
O	2.591211000000	-2.390893000000	-0.456358000000
H	-0.881619000000	-2.564696000000	1.212655000000
H	2.524857000000	-2.761442000000	-1.347479000000
C	0.893361000000	2.852039000000	1.611911000000
N	1.424455000000	1.903910000000	0.610385000000
C	2.815060000000	2.186602000000	0.195256000000
H	-0.128195000000	2.564351000000	1.844952000000
H	0.915116000000	3.854379000000	1.188240000000
H	1.514534000000	2.815770000000	2.504870000000
H	0.811016000000	1.920176000000	-0.233934000000
H	3.109168000000	1.432137000000	-0.529531000000
H	3.462873000000	2.149504000000	1.069036000000
H	2.849839000000	3.176796000000	-0.254921000000
O	0.041605000000	2.074551000000	-1.811055000000
H	-0.919915000000	2.172638000000	-1.803663000000
H	0.203656000000	1.151524000000	-2.057016000000
O	-1.327176000000	-2.046506000000	1.901547000000
H	-0.663604000000	-1.368636000000	2.100625000000
H	-2.463640000000	-1.248415000000	1.186276000000

**(SA)<sub>2</sub>(DMA)(W)<sub>3</sub>**

S	-1.471567000000	-1.477579000000	-0.073025000000
O	-0.179740000000	-2.095989000000	0.091438000000
O	-2.646275000000	-2.273592000000	-0.206335000000
O	-1.626417000000	-0.508319000000	1.138604000000
O	-1.414122000000	-0.530524000000	-1.309403000000
H	-2.623061000000	-0.114557000000	1.157031000000
H	-0.538264000000	0.021968000000	-1.261049000000

S	0.669077000000	1.762001000000	0.051008000000
O	-0.611930000000	2.424330000000	0.098310000000
O	0.735078000000	0.730300000000	-1.022457000000
O	1.846633000000	2.593580000000	0.064503000000
O	0.798657000000	0.899056000000	1.404921000000
H	3.354791000000	1.676534000000	-0.021866000000
H	-0.068840000000	0.477632000000	1.568175000000
C	2.624151000000	-1.771868000000	-1.374935000000
N	2.485758000000	-1.276391000000	0.012733000000
C	2.723160000000	-2.305867000000	1.044938000000
H	2.430601000000	-0.939761000000	-2.047205000000
H	1.890792000000	-2.560206000000	-1.530662000000
H	3.635074000000	-2.149029000000	-1.515667000000
H	1.528909000000	-0.920987000000	0.114879000000
H	2.587239000000	-1.852718000000	2.024360000000
H	3.738399000000	-2.684172000000	0.942652000000
H	1.999025000000	-3.105009000000	0.906193000000
O	4.049296000000	0.985403000000	0.023551000000
H	3.120200000000	-0.459360000000	0.144402000000
H	4.693341000000	1.300732000000	0.662838000000
O	-3.901963000000	0.414974000000	1.037386000000
H	-3.790969000000	1.031358000000	0.260885000000
H	-4.517561000000	-0.277061000000	0.771950000000
O	-3.160529000000	1.860060000000	-1.022968000000
H	-2.330765000000	2.248007000000	-0.694081000000
H	-2.862749000000	1.162790000000	-1.620107000000

**(SA)<sub>2</sub>(DMA)(W)<sub>4</sub>**

S	-1.436903000000	-0.276375000000	-1.175044000000
O	-2.637536000000	0.474565000000	-1.479912000000
O	-0.440473000000	0.083323000000	-2.355632000000
O	-0.777478000000	0.153800000000	0.059799000000
O	-1.614777000000	-1.736437000000	-1.190507000000
H	0.754624000000	1.795798000000	-0.372519000000
H	-0.949199000000	-2.326576000000	0.002421000000
S	2.252411000000	-0.733870000000	-0.198292000000
O	1.777842000000	-1.219004000000	1.112624000000
O	2.310447000000	0.711210000000	-0.279227000000
O	3.791364000000	-1.157313000000	-0.281276000000
O	1.585640000000	-1.412780000000	-1.297378000000
H	3.834640000000	-2.109246000000	-0.445484000000
H	0.375986000000	-0.445591000000	-2.201167000000
C	1.424663000000	3.466797000000	0.614358000000
N	0.341034000000	2.558693000000	0.185615000000
C	-0.759799000000	3.218482000000	-0.552824000000

H	2.182909000000	2.872314000000	1.116518000000
H	1.013548000000	4.220148000000	1.283500000000
H	1.853526000000	3.941778000000	-0.265417000000
H	-0.020135000000	2.042562000000	1.000650000000
H	-1.515256000000	2.474279000000	-0.796011000000
H	-0.354010000000	3.651758000000	-1.464550000000
H	-1.181283000000	4.001284000000	0.074896000000
O	-3.900246000000	-0.153869000000	0.980413000000
H	-3.612532000000	0.141782000000	0.097473000000
H	-4.635254000000	-0.752807000000	0.824437000000
O	-0.542081000000	-2.577775000000	0.920714000000
H	0.372023000000	-2.193384000000	0.924534000000
H	-1.094737000000	-1.983927000000	1.616192000000
O	0.418843000000	0.784556000000	2.485185000000
H	0.873257000000	0.878768000000	3.327520000000
H	0.940053000000	0.126929000000	1.976048000000
O	-1.785615000000	-1.088891000000	2.465527000000
H	-1.183293000000	-0.325358000000	2.518101000000
H	-2.566852000000	-0.760195000000	1.965115000000

**(SA)(TA)(AM)**

O	-2.885489000000	1.632262000000	-0.615311000000
O	-2.177851000000	-0.172077000000	1.525749000000
O	-0.035222000000	-0.424035000000	-1.102895000000
O	-4.605775000000	-1.148058000000	-0.904399000000
O	-0.236919000000	1.655333000000	-0.279558000000
O	-4.801992000000	-0.513226000000	1.235464000000
C	-2.210452000000	0.425561000000	-0.799221000000
C	-2.616834000000	-0.602063000000	0.270831000000
C	-0.706625000000	0.613132000000	-0.709797000000
C	-4.124848000000	-0.742013000000	0.272579000000
H	-2.456516000000	0.029120000000	-1.786164000000
H	-2.175427000000	-1.572866000000	0.019452000000
H	-2.355726000000	2.166695000000	-0.009329000000
H	-2.960260000000	-0.049118000000	2.081206000000
H	0.968443000000	-0.286646000000	-1.006856000000
H	-5.570008000000	-1.192367000000	-0.831163000000
S	3.273781000000	-0.654288000000	0.122278000000
O	2.800752000000	-1.968112000000	0.441725000000
O	2.459489000000	0.056460000000	-0.890092000000
O	3.550653000000	0.248496000000	1.243174000000
O	4.717597000000	-0.822719000000	-0.553535000000
H	2.820424000000	1.582954000000	0.919394000000
H	4.726443000000	-1.674279000000	-1.010293000000
N	2.281750000000	2.420598000000	0.512602000000

H	2.783449000000	2.729973000000	-0.317076000000
H	2.198946000000	3.183116000000	1.178670000000
H	1.338092000000	2.085549000000	0.208553000000

**(SA)(TA)(AM)(W)<sub>1</sub>**

O	-2.980219000000	1.438972000000	-0.972548000000
O	-2.013961000000	-0.074939000000	1.342182000000
O	-0.074805000000	-0.600427000000	-1.156299000000
O	-4.693590000000	-1.282544000000	-0.672121000000
O	-0.340756000000	1.625196000000	-1.005386000000
O	-4.642165000000	-0.311268000000	1.347790000000
C	-2.274017000000	0.237586000000	-1.041990000000
C	-2.581804000000	-0.632610000000	0.184661000000
C	-0.775275000000	0.490519000000	-1.075857000000
C	-4.082592000000	-0.717752000000	0.368496000000
H	-2.554251000000	-0.318483000000	-1.942098000000
H	-2.179887000000	-1.636212000000	0.021983000000
H	-2.326649000000	2.145578000000	-0.873734000000
H	-2.739491000000	0.243040000000	1.900614000000
H	0.927498000000	-0.404096000000	-1.136483000000
H	-5.646645000000	-1.269889000000	-0.502051000000
S	3.255495000000	-0.540605000000	-0.034916000000
O	2.580035000000	-1.454606000000	0.867007000000
O	2.379517000000	0.019025000000	-1.076845000000
O	4.022764000000	0.503711000000	0.626385000000
O	4.284157000000	-1.415651000000	-0.889641000000
H	2.870918000000	1.969758000000	0.503953000000
H	4.833587000000	-1.917837000000	-0.272261000000
N	1.897708000000	2.314135000000	0.559775000000
H	1.442488000000	2.222380000000	-0.356326000000
H	1.377589000000	1.634771000000	1.194625000000
H	1.847585000000	3.267733000000	0.903547000000
O	0.727898000000	0.368649000000	1.968250000000
H	-0.196995000000	0.140985000000	1.781089000000
H	1.263511000000	-0.422275000000	1.775319000000

**(SA)(TA)(AM)(W)<sub>2</sub>**

O	3.164992000000	-1.595941000000	0.879737000000
O	2.323240000000	1.176884000000	0.513970000000
O	0.209631000000	-0.811708000000	-0.936856000000
O	4.813154000000	-0.269373000000	-1.585930000000
O	0.533257000000	-1.609282000000	1.138096000000
O	4.941068000000	1.142454000000	0.150890000000
C	2.432149000000	-1.130007000000	-0.212245000000



C	2.791416000000	0.332996000000	-0.505702000000
C	0.939658000000	-1.213107000000	0.062726000000
C	4.297946000000	0.461214000000	-0.597006000000
H	2.653313000000	-1.726821000000	-1.102940000000
H	2.345571000000	0.626594000000	-1.459719000000
H	2.531267000000	-1.782906000000	1.586846000000
H	3.092462000000	1.478933000000	1.020316000000
H	-0.782292000000	-0.908237000000	-0.724886000000
H	5.775945000000	-0.170428000000	-1.559911000000
S	-3.323999000000	-0.246305000000	-0.507326000000
O	-2.210409000000	-1.190235000000	-0.282489000000
O	-3.008688000000	0.750365000000	-1.513353000000
O	-4.515882000000	-1.126132000000	-1.107392000000
O	-3.863185000000	0.248207000000	0.742688000000
H	-4.322725000000	-1.295802000000	-2.039269000000
H	-2.652160000000	-0.239779000000	2.011177000000
N	-1.699982000000	-0.363962000000	2.397191000000
H	-1.711985000000	-0.470271000000	3.406352000000
H	-1.118283000000	0.485414000000	2.100244000000
H	-1.261115000000	-1.173818000000	1.944430000000
O	-0.305941000000	1.701192000000	1.507504000000
H	0.573389000000	1.532735000000	1.135411000000
H	-0.802593000000	2.231261000000	0.846902000000
O	-1.846812000000	2.993613000000	-0.322602000000
H	-2.342529000000	2.303459000000	-0.800209000000
H	-1.536825000000	3.611330000000	-0.988611000000

**(SA)(TA)(AM)(W)<sub>3</sub>**

O	1.083870000000	-0.721972000000	1.489545000000
O	1.559938000000	0.413873000000	-1.241529000000
O	0.130144000000	-2.257385000000	-1.551491000000
O	4.220029000000	-1.149552000000	0.463659000000
O	-0.882388000000	-2.323867000000	0.438136000000
O	3.636181000000	1.001979000000	0.262332000000
C	1.360856000000	-1.469605000000	0.343989000000
C	2.201765000000	-0.690926000000	-0.682009000000
C	0.074374000000	-2.053869000000	-0.241674000000
C	3.417777000000	-0.156088000000	0.055059000000
H	1.962738000000	-2.328459000000	0.659549000000
H	2.545810000000	-1.390795000000	-1.451859000000
H	0.611184000000	0.099130000000	1.242657000000
H	0.601900000000	0.258755000000	-1.346933000000
H	-0.776617000000	-2.460350000000	-1.860751000000
H	4.947409000000	-0.750965000000	0.962338000000
S	-1.430782000000	1.506894000000	-0.050774000000

O	-1.125933000000	0.352061000000	-0.936669000000
O	-2.861637000000	1.609444000000	0.181005000000
O	-0.617861000000	1.436789000000	1.168810000000
O	-1.004332000000	2.796003000000	-0.802794000000
H	-1.387071000000	0.201736000000	2.556938000000
H	-0.004137000000	2.955779000000	-0.654023000000
N	-3.408774000000	-1.054201000000	0.747353000000
H	-3.007143000000	-1.629563000000	-0.001795000000
H	-4.326460000000	-1.399323000000	1.011308000000
H	-3.459217000000	-0.068712000000	0.419700000000
O	-1.637754000000	-0.719223000000	2.738445000000
H	-0.863329000000	-1.218010000000	2.431510000000
H	-2.742773000000	-1.045440000000	1.578290000000
O	-2.522899000000	-1.637487000000	-2.050197000000
H	-2.134522000000	-0.756705000000	-1.862309000000
H	-3.016194000000	-1.558231000000	-2.870882000000
O	1.506309000000	3.090631000000	-0.408429000000
H	1.908237000000	2.226554000000	-0.617225000000
H	1.696157000000	3.226281000000	0.525597000000

**(SA)(TA)(AM)(W)<sub>4</sub>**

O	2.498228000000	-0.564114000000	1.286650000000
O	3.478283000000	-1.279028000000	-1.376996000000
O	4.930750000000	1.428745000000	-0.390101000000
O	0.383762000000	0.429940000000	-0.983532000000
O	5.086015000000	-0.037575000000	1.299655000000
O	0.867355000000	-1.733661000000	-1.326395000000
C	2.944286000000	0.348198000000	0.317544000000
C	2.659326000000	-0.186351000000	-1.095276000000
C	4.437707000000	0.546543000000	0.478092000000
C	1.191092000000	-0.572949000000	-1.157177000000
H	2.441798000000	1.311049000000	0.452254000000
H	2.843617000000	0.615107000000	-1.816851000000
H	3.280051000000	-0.916829000000	1.738169000000
H	2.916653000000	-2.066727000000	-1.370003000000
H	5.887475000000	1.484263000000	-0.251463000000
H	-0.623899000000	0.142727000000	-0.905067000000
S	-2.666633000000	0.258207000000	0.507369000000
O	-2.002262000000	-0.197769000000	-0.752268000000
O	-1.744639000000	1.059053000000	1.311017000000
O	-3.853600000000	1.163493000000	0.057090000000
O	-3.269968000000	-0.851483000000	1.211112000000
H	-3.511611000000	2.028414000000	-0.341982000000
H	-1.118439000000	-2.317271000000	0.824138000000
N	-1.360412000000	-2.894656000000	-0.013279000000

H	-2.336917000000	-2.712688000000	-0.330960000000
H	-0.696666000000	-2.590708000000	-0.739775000000
H	-1.232496000000	-3.881550000000	0.191523000000
O	-3.981621000000	-2.460828000000	-0.952964000000
H	-4.211384000000	-1.959103000000	-0.153673000000
H	-3.839536000000	-1.771335000000	-1.612781000000
O	-0.382977000000	3.077697000000	-0.074376000000
H	0.137803000000	2.561627000000	-0.699503000000
H	-0.697557000000	2.413721000000	0.565539000000
O	-2.930013000000	3.377720000000	-0.914922000000
H	-3.326209000000	4.169265000000	-0.540447000000
H	-1.971505000000	3.411878000000	-0.692617000000
O	-0.223903000000	-1.297714000000	1.927479000000
H	0.700320000000	-1.059717000000	1.758697000000
H	-0.690218000000	-0.459305000000	2.069156000000

**(SA)(TA)(DMA)**

O	2.333570000000	-1.297011000000	1.472544000000
O	2.250533000000	1.230034000000	0.040466000000
O	-0.089407000000	-0.661177000000	-1.055375000000
O	4.594345000000	-1.277412000000	-0.906843000000
O	-0.237308000000	-0.942701000000	1.161491000000
O	4.785479000000	0.598763000000	0.305221000000
C	1.893771000000	-1.171541000000	0.151898000000
C	2.629418000000	-0.010787000000	-0.519859000000
C	0.386582000000	-0.915268000000	0.076742000000
C	4.121394000000	-0.178623000000	-0.322806000000
H	2.103230000000	-2.083092000000	-0.419868000000
H	2.395736000000	-0.010870000000	-1.586456000000
H	1.536852000000	-1.287071000000	2.023704000000
H	2.980018000000	1.509322000000	0.616112000000
H	-1.574799000000	-0.878906000000	-1.281346000000
H	5.537045000000	-1.347598000000	-0.697215000000
S	-3.312857000000	-0.565783000000	-0.091672000000
O	-4.703830000000	-0.790913000000	-0.239321000000
O	-2.586650000000	-1.032820000000	-1.380950000000
O	-2.846614000000	0.777829000000	0.217781000000
O	-2.766984000000	-1.513440000000	1.017115000000
H	-1.099132000000	1.191393000000	0.263835000000
H	-1.787897000000	-1.305960000000	1.158660000000
C	-0.667105000000	2.476784000000	-1.258602000000
N	-0.481655000000	2.012010000000	0.135693000000
C	-0.869268000000	3.012446000000	1.153305000000
H	-0.350318000000	1.675492000000	-1.921956000000
H	-0.067033000000	3.370530000000	-1.418404000000

H	-1.724271000000	2.686513000000	-1.406776000000
H	0.496470000000	1.709193000000	0.260478000000
H	-0.702802000000	2.588400000000	2.140675000000
H	-1.927122000000	3.231203000000	1.024300000000
H	-0.272506000000	3.912616000000	1.020068000000

**(SA)(TA)(DMA)(W)<sub>1</sub>**

O	0.805909000000	-0.104089000000	-1.125020000000
O	1.389294000000	-0.969954000000	1.620005000000
O	3.799018000000	-1.824057000000	-0.481500000000
O	-0.814778000000	-2.815610000000	-0.474808000000
O	3.309416000000	0.358743000000	-0.460325000000
O	-1.118178000000	-1.795414000000	1.493633000000
C	1.526171000000	-1.237549000000	-0.758186000000
C	1.080067000000	-1.855513000000	0.578251000000
C	2.962397000000	-0.784660000000	-0.564627000000
C	-0.412433000000	-2.158823000000	0.571424000000
H	1.495171000000	-2.015019000000	-1.527639000000
H	1.610138000000	-2.809169000000	0.699252000000
H	-0.172070000000	-0.246010000000	-1.185886000000
H	0.639545000000	-0.984736000000	2.231467000000
H	4.683856000000	-1.478479000000	-0.295707000000
H	-1.838262000000	-2.765526000000	-0.525782000000
S	-2.181605000000	1.167817000000	-0.181251000000
O	-3.570301000000	1.172639000000	0.175095000000
O	-1.824335000000	-0.007167000000	-1.014715000000
O	-1.600276000000	2.405361000000	-0.672722000000
O	-1.321246000000	0.954686000000	1.180912000000
H	0.052625000000	2.533708000000	0.100562000000
H	-1.471491000000	0.044388000000	1.493066000000
C	1.788850000000	3.141553000000	-0.831095000000
N	1.063231000000	2.313886000000	0.155064000000
C	1.575307000000	2.421802000000	1.534655000000
H	1.334774000000	2.980359000000	-1.806243000000
H	2.829860000000	2.828625000000	-0.846791000000
H	1.703288000000	4.189177000000	-0.548503000000
H	1.115884000000	1.324084000000	-0.160554000000
H	0.931682000000	1.831486000000	2.180743000000
H	1.562878000000	3.466690000000	1.840223000000
H	2.589230000000	2.027592000000	1.554484000000
O	-3.288738000000	-2.294380000000	-0.710700000000
H	-3.069689000000	-1.364314000000	-0.924242000000
H	-3.782791000000	-2.252049000000	0.114725000000

**(SA)(TA)(AM)(W)<sub>2</sub>**

O	-2.646708000000	-0.133286000000	1.366047000000
O	-3.268412000000	1.434855000000	-1.039582000000
O	-5.356193000000	-1.020252000000	-0.773743000000
O	-0.662241000000	-0.982633000000	-0.967132000000
O	-5.284068000000	0.026839000000	1.207143000000
O	-0.627373000000	1.262129000000	-0.984736000000
C	-3.225343000000	-0.632717000000	0.189197000000
C	-2.731352000000	0.146035000000	-1.037008000000
C	-4.730991000000	-0.499205000000	0.282710000000
C	-1.211680000000	0.199141000000	-0.997963000000
H	-2.964925000000	-1.687877000000	0.071588000000
H	-3.034526000000	-0.396199000000	-1.938875000000
H	-3.335553000000	0.343425000000	1.852691000000
H	-2.523760000000	2.047560000000	-0.958979000000
H	-6.305151000000	-0.861977000000	-0.665809000000
H	0.347594000000	-0.917616000000	-0.928633000000
S	2.750220000000	-1.460471000000	0.055913000000
O	1.892044000000	-0.755014000000	-0.908548000000
O	2.130652000000	-1.662574000000	1.352641000000
O	2.881862000000	-2.909573000000	-0.615549000000
O	4.082529000000	-0.887246000000	0.112819000000
H	3.343704000000	-3.486781000000	0.007694000000
H	4.207129000000	0.639155000000	-0.968803000000
C	2.816252000000	1.812256000000	1.500751000000
N	1.817515000000	1.880485000000	0.408641000000
C	1.562857000000	3.256199000000	-0.061796000000
H	2.920037000000	0.777107000000	1.818162000000
H	2.459458000000	2.419442000000	2.330385000000
H	3.765617000000	2.185762000000	1.123172000000
H	0.949479000000	1.413266000000	0.736824000000
H	0.810493000000	3.217479000000	-0.844053000000
H	2.497373000000	3.659247000000	-0.447174000000
H	1.207334000000	3.855108000000	0.774564000000
O	3.970574000000	1.496351000000	-1.367264000000
H	3.880451000000	1.313367000000	-2.306308000000
H	2.165120000000	1.328492000000	-0.387456000000
O	0.152362000000	0.276531000000	1.883310000000
H	-0.780201000000	0.042281000000	1.771306000000
H	0.665525000000	-0.546374000000	1.826007000000

**(SA)(TA)(DMA)(W)<sub>3</sub>**

O	2.769987000000	-1.289852000000	-0.736750000000
O	4.005244000000	1.392521000000	-0.729729000000
O	5.793753000000	-0.606403000000	1.026473000000

O	1.214146000000	0.487113000000	1.279421000000
O	5.394779000000	-1.620955000000	-0.932600000000
O	1.416102000000	1.866755000000	-0.479474000000
C	3.543779000000	-0.736508000000	0.292772000000
C	3.364635000000	0.786503000000	0.351677000000
C	5.005215000000	-1.048244000000	0.045073000000
C	1.879091000000	1.102870000000	0.347740000000
H	3.241044000000	-1.168630000000	1.250300000000
H	3.785476000000	1.150340000000	1.295880000000
H	3.368906000000	-1.551534000000	-1.451503000000
H	3.327648000000	1.846116000000	-1.250658000000
H	6.710239000000	-0.797676000000	0.779691000000
H	0.219975000000	0.701724000000	1.222039000000
S	-1.879360000000	1.427492000000	-0.149083000000
O	-1.270947000000	1.046824000000	1.154163000000
O	-1.598834000000	0.433128000000	-1.175282000000
O	-3.284971000000	1.747897000000	-0.008453000000
O	-1.179137000000	2.770631000000	-0.572835000000
H	-4.044875000000	0.089532000000	-0.223371000000
H	-0.214005000000	2.584144000000	-0.631961000000
C	-5.428640000000	-1.388888000000	0.232907000000
N	-4.225302000000	-0.898991000000	-0.468256000000
C	-4.295136000000	-1.028166000000	-1.939524000000
H	-5.275402000000	-1.249614000000	1.299721000000
H	-5.556054000000	-2.446401000000	0.008389000000
H	-6.299174000000	-0.828942000000	-0.104749000000
H	-3.395373000000	-1.455182000000	-0.108501000000
H	-3.377761000000	-0.622859000000	-2.358043000000
H	-5.156669000000	-0.473025000000	-2.306866000000
H	-4.396037000000	-2.082340000000	-2.191681000000
O	-3.165326000000	-0.532521000000	2.431534000000
H	-2.534754000000	0.142400000000	2.116786000000
H	-3.377494000000	-0.291954000000	3.336714000000
O	-2.335295000000	-2.471177000000	0.599515000000
H	-2.325789000000	-2.076974000000	1.483521000000
H	-1.432531000000	-2.366860000000	0.228674000000
O	-0.074747000000	-1.851829000000	-0.739593000000
H	-0.397531000000	-0.971321000000	-0.989236000000
H	0.885337000000	-1.780330000000	-0.657011000000

**(SA)(TA)(DMA)(W)<sub>4</sub>**

O	1.165141000000	-0.615074000000	1.368668000000
O	1.735338000000	0.541100000000	-1.181687000000
O	0.661591000000	-2.539886000000	-1.580944000000
O	4.472839000000	-1.042603000000	0.382021000000

O	-0.671096000000	-2.175060000000	0.170147000000
O	3.847087000000	1.102957000000	0.321477000000
C	1.595362000000	-1.402213000000	0.294378000000
C	2.428947000000	-0.571019000000	-0.699773000000
C	0.403112000000	-2.080218000000	-0.382077000000
C	3.641986000000	-0.043366000000	0.043729000000
H	2.233848000000	-2.198086000000	0.689171000000
H	2.776855000000	-1.225173000000	-1.505207000000
H	0.522841000000	0.024498000000	1.004838000000
H	0.895997000000	0.286995000000	-1.626660000000
H	-0.231690000000	-2.713043000000	-2.032738000000
H	5.210551000000	-0.653496000000	0.872660000000
S	-1.657497000000	0.619834000000	-1.042652000000
O	-0.776790000000	0.174284000000	-2.136139000000
O	-2.736861000000	-0.307998000000	-0.760099000000
O	-0.868636000000	0.980528000000	0.147422000000
O	-2.357303000000	1.945332000000	-1.506596000000
H	-1.267199000000	0.231795000000	2.298754000000
H	-1.670350000000	2.672109000000	-1.476705000000
C	-1.627272000000	-1.632049000000	3.103723000000
N	-1.941469000000	-0.546570000000	2.154152000000
C	-3.315920000000	-0.011988000000	2.256842000000
H	-0.602882000000	-1.946831000000	2.918301000000
H	-2.308991000000	-2.462778000000	2.932774000000
H	-1.738421000000	-1.255963000000	4.119180000000
H	-1.773778000000	-0.884890000000	1.195881000000
H	-3.432584000000	0.768788000000	1.510323000000
H	-3.462287000000	0.383982000000	3.260062000000
H	-4.023264000000	-0.813533000000	2.055407000000
O	-1.700666000000	-2.453618000000	-2.595367000000
H	-2.196969000000	-2.297562000000	-1.776965000000
H	-1.559123000000	-1.544097000000	-2.905729000000
O	1.317508000000	2.631148000000	0.645850000000
H	2.222357000000	2.909141000000	0.825957000000
H	1.433949000000	1.856779000000	0.057657000000
O	-0.404870000000	3.706414000000	-1.310800000000
H	0.143283000000	3.442231000000	-0.547102000000
H	0.188260000000	3.694183000000	-2.067749000000
O	-0.055048000000	1.440602000000	2.891729000000
H	0.761456000000	0.985848000000	3.127669000000
H	0.205214000000	1.987869000000	2.127187000000