Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Computational Study of the Rayleigh Light Scattering Properties of Atmospheric Pre-Nucleation Clusters

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Basis set and functional assessment of polarizabilities

Calculated polarizabilities are very dependent on diffuse functions and the choice of DFT functional. To assess the performance of different functionals and basis sets preliminary results are benchmarked against coupled cluster ccsd(t) and experimental results. All calculations were done in Gaussian09.

Table 1: Calculated isotropic mean polarizabilities ($\bar{\alpha}$) of H_2O using different DFT functionals and basis sets compared to coupled cluster and experimental data.

Basis set	CC2	CCSD	CCSD(T)	CAM-B3LYP	B3LYP	M06-2X	PW91
cc-pvdz	5.12	5.13	5.15	5.24	5.29	5.19	5.40
cc-pvtz	6.87	6.90	6.95	7.01	7.08	6.97	7.26
cc-pvqz	7.73	9.32	7.87	7.93	8.01	7.89	8.21
aug-cc-pvdz	8.87	8.99	9.14	9.27	9.39	8.85	9.88
aug-cc-pvtz	9.15	9.26	9.46	9.62	9.77	9.20	10.32
aug-cc-pvqz	9.21	9.32	9.54	9.75	9.90	9.42	10.44
d-aug-cc-pvdz	8.87	9.53	9.70	9.86	10.02	9.32	10.61
d-aug-cc-pvtz	9.31	9.44	9.65	9.85	10.01	9.37	10.65
d-aug-cc-pvqz	9.26	9.38	9.61	9.84	10.00	9.48	10.58
Exp							**9.92**

Table 2: Calculated isotropic mean polarizabilities ($\bar{\alpha}$) of NH_3 using different DFT functionals and basis sets compared to coupled cluster and experimental data.

Basis set	CC2	CCSD	CCSD(T)	CAM-B3LYP	B3LYP	M06-2X	PW91
cc-pvdz	8.39	8.41	8.44	8.58	8.66	8.53	8.79
cc-pvtz	10.68	10.71	10.78	10.89	11.00	10.86	11.25
cc-pvqz	11.83	11.87	12.00	12.08	12.22	12.07	12.49
aug-cc-pvdz	13.48	13.61	13.81	13.91	14.16	13.54	14.74
aug-cc-pvtz	13.69	13.81	14.06	14.26	14.54	13.79	15.21
aug-cc-pvqz	13.70	13.81	14.11	14.34	14.64	14.03	15.32
d-aug-cc-pvdz	13.92	14.09	14.32	14.45	14.77	13.96	15.51
d-aug-cc-pvtz	13.80	13.93	14.19	14.41	14.73	13.92	15.47
d-aug-cc-pvqz	13.73	13.85	14.16	14.40	14.71	14.07	15.42
Exp							**14.21**

Table 3: Calculated isotropic mean polarizabilities ($\bar{\alpha}$) of H_2SO_4 using different DFT functionals and basis sets compared to coupled cluster and experimental data.

Basis set	CC2	CCSD	CCSD(T)	CAM-B3LYP	B3LYP	M06-2X	PW91
cc-pvdz	24.98	25.20	25.52	25.43	25.85	25.23	26.75
cc-pvtz	29.47	29.72	30.19	30.05	30.48	29.87	31.53
cc-pvqz	31.93	32.20	32.92	32.66	33.11	32.40	34.20
aug-cc-pvdz	34.31	34.80	35.46	35.04	35.59	34.13	37.31
aug-cc-pvtz	34.32	34.72	35.24	35.78	34.51	37.41	
aug-cc-pvqz	-	-	-	35.29	35.82	34.63	37.33
d-aug-cc-pvdz	34.97	35.48	36.19	35.71	36.27	34.71	38.00
d-aug-cc-pvtz	34.47	34.88	35.87	35.41	35.95	34.63	37.58
d-aug-cc-pvqz	-	-	-	35.32	35.85	34.65	37.41
Exp							-

Cluster Structures

Minimum identified clusters within each cluster morphology [Site 1 - Site 2] optimized at the M06-2X/6-311++G(3df,3pd) level of theory. The relative stability within each cluster morphology is shown in the brackets () in kcal/mol. The mean anisotropic ($\Delta\alpha$) and isotropic ($\bar{\alpha}$) polarizabilities are calculated at the CAM-B3LYP/aug-cc-pvdz level of theory.

$(H_2SO_4)(H_2O)$ [0-1] Cluster (0.00), $\Delta\alpha$ = 10.94, $\bar{\alpha}$ = 44.60

O 2.66843900 -0.04455000 -0.05534900
H 3.16246700 0.75743900 -0.23878000
H 2.25824500 0.07595000 0.81242100
S -0.57806500 -0.09464700 0.10319800
O -1.79268900 -0.81554500 0.04316100
O 0.19956100 -0.02061200 1.29299900
O 0.32089900 -0.57631800 -1.06039500
H 1.27738600 -0.37508200 -0.84624900
O -0.87453100 1.40877000 -0.28129400
H -1.62248300 1.44207300 -0.89154200

$(H_2SO_4)(H_2O)_2$ [0-2] Cluster (0.55 kcal/mol), $\Delta\alpha$ = 11.64, $\bar{\alpha}$ = 54.46

O 2.50005300 -1.20457100 -0.09324600
H 1.61435500 -1.36236700 -0.45686000
H 2.58640100 -1.78335300 0.66647700
O 2.05592000 1.40869500 0.15232200
H 2.50129700 1.86991400 -0.56209500
H 2.35312900 0.46892100 0.11263800
S -0.97067900 -0.05670800 -0.12863000
O -2.36472600 -0.01219200 -0.35997500
O -0.10839900 -0.80711200 -0.98319200
O -0.45911000 1.37803000 0.01730500
H 0.57244900 1.41933800 0.05839000
O -0.71084100 -0.67831600 1.30728800
H -1.39994300 -0.38139400 1.91552100

$(H_2SO_4)(H_2O)_2$ [1-1] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 18.46, $\bar{\alpha}$ = 54.34

O -3.05163600 -0.73526600 0.07231000
H -3.83442900 -0.58262300 -0.46085800
H -2.84004200 0.10542500 0.50264700
O 3.08645500 -0.63479300 0.10039600

H 2.83772000 0.05096500 -0.53533900
H 3.39105300 -1.38660100 -0.41198800
S 0.00107300 0.38036400 -0.02366000
O -1.04810300 1.14104200 0.56954700
O 1.01090100 1.02404000 -0.79648900
O 0.67865800 -0.42252300 1.11507100
H 1.61172300 -0.65289600 0.84776500
O -0.62782800 -0.71516800 -0.92599300
H -1.57076600 -0.87875000 -0.64239200

$(H_2SO_4)(H_2O)_3$ [0-3] Cluster (1.48 kcal/mol), $\Delta\alpha$ = 13.69, $\bar{\alpha}$ = 63.52

O -1.50695300 -1.37165700 -1.16324800
H -1.97182900 -1.32823000 -0.31412000
H -1.77394500 -0.56697200 -1.62131000
O -2.32533600 -0.35004400 1.33603200
H -2.80419200 -0.52245500 2.14802600
H -1.37303500 -0.30824600 1.55172100
O -1.87651300 1.46659500 -0.65400000
H -2.24402600 2.35156800 -0.70226900
H -2.22494000 1.04912900 0.15415400
S 1.24418200 0.02923400 0.16193500
O 0.32203500 -0.02795800 1.26628600
O 2.62090400 0.18411800 0.41414100
O 1.05611300 -1.23222300 -0.70862400
H 0.08225700 -1.37210200 -0.91148100
O 0.78417900 1.19212900 -0.76566200
H -0.19263700 1.34187600 -0.69509200

$(H_2SO_4)(H_2O)_3$ [1-2] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 20.10, $\bar{\alpha}$ = 64.35

O 3.36111200 -0.59223100 0.51322700
H 3.97860300 -1.08118200 -0.03329600
H 2.51146400 -1.05780400 0.45341400
O 2.20598100 1.68653600 -0.22848800
H 2.14571500 2.26192400 0.53717400
H 2.76528400 0.91929000 0.03659600
O -3.40535200 0.61362000 0.50771200
H -3.26630500 -0.03731500 -0.19539000
H -3.72748900 1.40928000 0.07920900
S -0.42960700 -0.44315400 -0.18247600
O 0.69717800 -1.25566300 0.14309700
O -1.55870300 -1.03751000 -0.81753500
O -0.88324000 0.21906600 1.15107100
H -1.82978600 0.51338700 1.05671100
O 0.00873600 0.74243700 -1.05534300
H 0.89053100 1.15284000 -0.72471500

$(H_2SO_4)(H_2O)_4$ [0-4] Cluster (3.73 kcal/mol), $\Delta\alpha$ = 11.15, $\bar{\alpha}$ = 73.13

O -1.92274200 -1.89320000 -0.30399400
H -2.03338300 -2.84521100 -0.34541800
H -1.03636400 -1.68268100 -0.65850000
O -1.30909000 -0.40611000 1.78657300
H -1.49527900 0.55689100 1.42351400
H -1.70419400 -1.04166500 1.13497400

S 1.39355000 -0.15830900 -0.10870200
O 0.33013900 -0.59862400 -0.99718500
O 2.72946400 -0.42025300 -0.51592300
O 1.22081600 1.44842300 -0.14461500
H 2.10034200 1.84320800 -0.11625900
O 1.10299500 -0.52741300 1.28145900
H -0.26607100 -0.50449200 1.65349300
O -1.56461900 1.85203900 0.75048800
H -1.85143600 1.61282300 -0.16172700
H -0.65485000 2.15721200 0.64197100
O -2.04123100 0.79336900 -1.67232800
H -2.58257100 0.00457700 -1.56679200
H -1.13885100 0.44642700 -1.74183500

$(H_2SO_4)(H_2O)_4$ [1-3] Cluster (1.32 kcal/mol), $\Delta\alpha$ = 19.88, $\bar{\alpha}$ = 73.25

O -3.16166500 -0.75937400 -0.39486500
H -3.80029800 -1.41220100 -0.68568100
H -2.28170900 -1.11347300 -0.60121700
O -1.83183100 0.66711700 1.62202100
H -1.85712300 1.29757700 0.86752100
H -2.51328400 0.02511900 1.37456100
O 3.44243500 1.04232400 -0.05361100
H 3.74217900 1.37288000 0.79622400
H 3.47557100 0.07661000 0.00234700
S 0.69425300 -0.62382700 -0.09193100
O -0.45921200 -1.11646400 -0.77948100
O 1.92285900 -1.33772100 -0.19059400
O 0.90834600 0.82357800 -0.65100100
H 1.84053700 1.11396700 -0.44011800
O 0.38619500 -0.41106100 1.38516700
H -0.56289800 0.03806300 1.52927500
O -1.91110300 1.82535200 -0.82436700
H -2.48283500 1.10128400 -1.11052600
H -1.03638300 1.61141200 -1.16764800

$(H_2SO_4)(H_2O)_4$ [2-2] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 23.62, $\bar{\alpha}$ = 74.46

O -3.80080400 -0.45444500 -0.46701700
H -4.39750100 -1.04523000 -0.00455300
H -2.96056500 -0.93251100 -0.56188500
O -2.54067000 1.58267100 0.69284000
H -2.49792700 2.30148900 0.05857400
H -3.13627400 0.90088400 0.30260900
O 2.54105700 1.58238100 -0.69285400
H 3.13625100 0.90035000 -0.30217600
H 2.49874200 2.30163200 -0.05905700
S 0.00004000 -0.53509700 -0.00001700
O -1.15827100 -1.27070700 -0.39481800
O 1.15834600 -1.27092100 0.39445600
O 0.33740200 0.41127800 -1.16714800
H 1.21436500 0.91105400 -0.99485200
O -0.33729700 0.41065700 1.16762900
H -1.21394300 0.91075200 0.99530700
O 3.80010200 -0.45455000 0.46698600

H 2.96007700 -0.93311300 0.56152200
H 4.39720500 -1.04467300 0.00419900

$(H_2SO_4)(H_2O)_5$ [0-5] Cluster (4.14 kcal/mol), $\Delta\alpha$ = 19.93, $\bar{\alpha}$ = 83.18

O 1.28653000 1.89392300 -0.85663300
H 1.39140100 2.66438400 -1.41776100
H 0.32553900 1.78061800 -0.70420400
O 0.84028000 -0.84301400 1.33963100
H 0.95569200 -1.03726000 0.37440800
H 1.53244700 -0.09852200 1.50598800
S -2.01698000 0.07416400 0.05990700
O -1.20989700 1.02915000 -0.66106700
O -3.42813500 0.22671900 0.01184400
O -1.66824500 -1.29597000 -0.73598300
H -2.36349300 -1.93991200 -0.55626000
O -1.50009200 -0.16993100 1.41849800
H -0.18664300 -0.51366000 1.44638700
O 1.17502100 -0.87972900 -1.31593200
H 1.24774700 0.08677800 -1.41182600
H 0.28586500 -1.10422800 -1.61910200
O 2.65277400 0.90241200 1.36559300
H 2.30482500 1.51537400 0.69678900
H 3.31331500 0.37484800 0.88534000
O 3.83694000 -0.88017100 -0.41758500
H 3.08382200 -1.21019600 -0.92399900
H 4.49974300 -1.57196600 -0.42121700

$(H_2SO_4)(H_2O)_5$ [1-4] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 18.46, $\bar{\alpha}$ = 82.99

O -2.11176200 1.34149200 -1.50091000
H -2.13259000 1.84149100 -2.31879900
H -1.31995200 0.76897900 -1.53194200
O -1.85609800 -0.48400300 1.72039900
H -1.74279100 0.52194500 1.57586100
H -2.39705800 -0.81264200 0.92744400
S 0.86466300 -0.59679700 -0.16368500
O -0.25643700 -0.57604000 -1.08988300
O 2.07707800 -1.17412600 -0.66376500
O 1.16366600 0.94696600 0.08613400
H 2.14596900 1.07881500 0.16686100
O 0.46145600 -1.13479500 1.13893900
H -0.88240600 -0.83859700 1.54963800
O -1.34435900 1.93391200 1.10757100
H -1.71300000 2.01297600 0.21109400
H -0.38805900 1.88130000 0.96297600
O -2.94887000 -1.21367300 -0.49185100
H -3.16576600 -0.38035200 -0.93269600
H -2.10032100 -1.45322900 -0.89443500
O 3.79636800 0.82420500 0.14344200
H 3.66224500 -0.06946400 -0.20940800
H 4.35078800 1.28603600 -0.48823200

$(H_2SO_4)(H_2O)_5$ [2-3] Cluster (2.14 kcal/mol), $\Delta\alpha$ = 22.45, $\bar{\alpha}$ = 83.45

O -3.57936300 0.44693600 -1.06903200

H -4.20448100 0.25393800 -1.76921000
H -2.76149100 -0.03354200 -1.28230100
O -2.64773500 0.18345600 1.57286100
H -2.32552300 1.07097900 1.30786400
H -3.34044600 0.01123700 0.91917300
S -0.04594100 -0.85921200 -0.23360700
O -1.04828400 -0.58991300 -1.22199100
O 0.99593900 -1.78069800 -0.53976100
O 0.59005900 0.52207000 0.10381800
H 1.55040000 0.37856600 0.42618400
O -0.70459100 -1.30521200 1.06921600
H -1.53147000 -0.71103700 1.31097100
O -1.76117200 2.34785600 0.16304100
H -2.36496900 2.06887700 -0.53723600
H -0.89605600 2.00951400 -0.09540500
O 2.93552000 -0.14295200 0.78424300
H 2.85782900 -1.03006800 0.41101500
H 3.70562100 0.27678200 0.36599200
O 5.12893500 1.09955500 -0.39783700
H 5.75562000 1.57298300 0.15314500
H 5.01557600 1.63038500 -1.18893700

$(H_2SO_4)(H_2O)_6$ [0-6] Cluster (11.71 kcal/mol), $\Delta\alpha = 20.28$, $\bar{\alpha} = 92.05$

O 1.36857300 -0.47891100 -1.44147600
H 0.65041000 -0.84104500 -1.96909500
H 1.03983600 -0.53753700 -0.52279000
O -0.06458800 1.93523100 -0.31663500
H 0.31592400 1.34193100 0.37123400
H 0.19363900 1.49951900 -1.13924100
S -2.48460700 -0.28152900 -0.08916000
O -1.40907800 -0.76472200 -0.88744600
O -3.80996000 -0.73921700 -0.27221100
O -2.04789400 -0.63433300 1.40160200
H -2.82029300 -0.57619200 1.97901900
O -2.49191500 1.25084600 -0.09259600
H -1.53241800 1.61548800 -0.18539200
O 0.84656100 -0.06119600 1.21507200
H 1.78531800 -0.14482400 1.54034200
H 0.24212300 -0.54997600 1.77755500
O 3.02071800 1.76418600 -0.47668700
H 2.33781200 2.43277300 -0.37496600
H 2.63992300 1.10384600 -1.06908000
O 3.41514200 -0.10831300 1.61768800
H 3.71490900 -0.82677400 1.03896000
H 3.53695000 0.68326900 1.07030300
O 3.75801200 -1.73994100 -0.62667700
H 2.95585200 -1.48011000 -1.10357000
H 4.00915000 -2.60493400 -0.95180200

$(H_2SO_4)(H_2O)_6$ [1-5] Cluster (3.81 kcal/mol), $\Delta\alpha = 25.43$, $\bar{\alpha} = 92.72$

O -2.15543100 -1.32901800 -0.93887600
H -1.52365000 -2.00566300 -1.19751100
H -1.74975000 -0.47766400 -1.21987200

O -1.29654300 -0.56659800 1.59830900
H -1.77681000 0.27864200 1.61017900
H -1.59866600 -1.00243600 0.77740000
S 1.63805000 -0.60699200 0.04174800
O 0.69716200 -1.37537900 -0.70345700
O 3.01666800 -0.97676500 0.04933600
O 1.54448400 0.85382400 -0.53707500
H 2.42605900 1.31008800 -0.43757200
O 1.17256500 -0.46041700 1.48351100
H 0.11954900 -0.48142500 1.55793000
O -1.25834200 1.18437500 -1.32641000
H -1.66159300 1.62631700 -0.56656400
H -0.30472300 1.22354000 -1.18657700
O -4.51795000 -0.08594000 -0.33045300
H -3.85695100 -0.74297800 -0.60771400
H -4.96624300 0.18395600 -1.13409500
O 4.02762300 1.60372700 -0.17431400
H 4.22789800 0.66801200 -0.02327400
H 4.58687100 1.89020200 -0.89928000
O -2.88388900 1.63128600 0.95777700
H -3.59803400 1.10441100 0.53631500
H -3.30352000 2.30410200 1.49588300

$(H_2SO_4)(H_2O)_6$ [2-4] Cluster (4.00 kcal/mol), $\Delta\alpha = 26.09$, $\bar{\alpha} = 93.69$

O -3.16080500 0.18609400 -1.37850800
H -3.52253500 0.14276100 -2.26554500
H -2.24469600 -0.14937600 -1.43753100
O -1.58297900 -0.00790200 1.83999600
H -1.71751900 0.85901700 1.38825000
H -2.38987500 -0.53057400 1.64075100
S 0.63878000 -0.40921400 -0.55672000
O -0.56084800 -0.53810800 -1.33308500
O 1.82709700 -1.00852000 -1.08260500
O 0.86471200 1.12690000 -0.41858100
H 1.78815300 1.32922700 -0.02591200
O 0.43515100 -0.90037400 0.85299500
H -0.50807700 -0.52064700 1.32337200
O -1.83001600 2.13757300 0.23483700
H -2.41191100 1.75784500 -0.43825600
H -0.94632200 2.11357600 -0.15296000
O 3.17987300 1.56376300 0.54167800
H 3.62291900 0.68989900 0.63561300
H 3.73846200 2.08939500 -0.03485700
O -3.84389400 -1.18652700 0.94179000
H -3.82572100 -0.76832900 0.06451500
H -4.68976500 -0.96590700 1.33482900
O 4.01547700 -0.97914200 0.62016100
H 3.31069800 -1.26303500 0.01479000
H 4.82556100 -1.38649400 0.31104300

$(H_2SO_4)(H_2O)_6$ [3-3] Cluster (0.00 kcal/mol), $\Delta\alpha = 23.37$, $\bar{\alpha} = 92.56$

O 3.74429800 -0.74218900 -0.67479900
H 4.35907600 -1.20804200 -1.24348100

H 2.85045800 -0.95907700 -0.98693300
O 2.57307800 1.61623200 0.28552700
H 2.57248200 1.01736600 1.06679900
H 3.21295700 1.18563500 -0.30044100
S -0.06108100 -0.19038300 -0.57972900
O 1.03103100 -0.98464200 -1.05546100
O -1.32204100 -0.32082300 -1.26441800
O -0.24797800 -0.50205000 0.90161700
H -1.24501400 -0.19258500 1.28165300
O 0.30128700 1.29736100 -0.64219700
H 1.27796700 1.47299700 -0.26516700
O 2.52536500 -0.50860500 1.95234400
H 1.62188400 -0.82088200 1.82184400
H 3.06003200 -0.99059700 1.30871100
O -3.41284900 -1.75597800 -0.01304000
H -2.76871800 -1.46750700 -0.67630100
H -4.23297900 -1.92934200 -0.47717000
O -2.68538800 2.04333100 -0.30184800
H -2.31773500 1.40692500 -0.93170500
H -2.04484800 2.75870700 -0.28291900
O -2.46731000 0.15221500 1.63861700
H -2.65792000 0.95872300 1.11248100
H -3.02629500 -0.54500800 1.23754400

$(H_2SO_4)(H_2O)_7$ [0-7] Cluster (1.30 kcal/mol), $\Delta\alpha = 14.69$, $\bar{\alpha} = 101.88$

O 0.24550500 2.14954100 -0.21150000
H -0.62064200 2.59043100 -0.35005600
H 0.15654100 1.30180800 -0.67426700
O 0.52273700 0.97002600 2.06746800
H 1.49457200 0.46278800 1.89436200
H 0.39862400 1.56757400 1.26289100
S -1.56114300 -0.77640200 0.00817300
O -0.27911800 -0.63828500 -0.67974600
O -2.62002200 0.02067700 -0.54910500
O -1.92037900 -2.29699100 -0.27769500
H -2.80696500 -2.48561300 0.05401100
O -1.42330400 -0.65906100 1.44983200
H -0.21758900 0.30654600 1.98244900
O 1.81405500 -2.23524500 0.09765900
H 1.60569300 -3.13229500 0.36570800
H 0.96845700 -1.80353900 -0.12707800
O 2.66041900 -0.05355500 1.54541000
H 2.50544900 -0.93644500 1.15968600
H 2.94964100 0.52147800 0.78635000
O 2.18455800 -0.56608800 -2.24688800
H 1.22129300 -0.57149300 -2.21762600
H 2.42865800 -1.34061500 -1.72597100
O 3.06129200 1.47863000 -0.57115800
H 2.82914400 0.86429700 -1.29230000
H 2.35593100 2.13588600 -0.56648700
O -2.33723400 2.80335800 -0.62727300
H -2.63137200 1.87727300 -0.61675000
H -2.92723200 3.28029300 -0.04170900

$(H_2SO_4)(H_2O)_7$ [1-6] Cluster (3.16 kcal/mol), $\Delta\alpha$ = 24.81, $\bar{\alpha}$ = 102.93

O -2.01792100 -1.96075200 -0.98839300
H -1.15107400 -1.64113000 -1.28704300
H -2.66155900 -1.29726700 -1.29363300
O -1.66904900 -1.50047400 1.47229800
H -2.25915300 -0.67567500 1.57485900
H -1.83292700 -1.79245900 0.49698200
S 1.34672100 -0.58959100 0.14623700
O 0.35174700 -0.49676200 -0.91893300
O 2.37917500 -1.55644900 -0.09829200
O 2.05688000 0.82727900 0.18557500
H 2.98751700 0.74077900 -0.15952400
O 0.70510800 -0.69198200 1.45346200
H -0.68398800 -1.19371800 1.51993400
O -1.45317200 1.54627400 -0.57192000
H -0.90952700 2.32311200 -0.34343600
H -0.80018600 0.83840000 -0.74251600
O -3.07664600 0.61559400 1.38987200
H -2.48620500 1.08876800 0.76328300
H -3.87573200 0.45163500 0.87750200
O 4.45391100 0.15446800 -0.64461900
H 4.11288300 -0.75162300 -0.57836000
H 4.73650400 0.27299200 -1.55354600
O 0.52815700 3.23950100 0.28253800
H 0.49663300 3.61167900 1.16578100
H 1.15157200 2.49963500 0.33260800
O -3.66503000 0.26903900 -1.48680200
H -2.96655500 0.94343100 -1.41745200
H -4.15102400 0.44900800 -2.29351700

$(H_2SO_4)(H_2O)_7$ [2-5] Cluster (1.98 kcal/mol), $\Delta\alpha$ = 24.54, $\bar{\alpha}$ = 103.13

O 0.94010300 -0.76417000 2.28293400
H 0.84129600 -1.14833500 3.15579000
H 0.06085400 -0.80982600 1.82702200
O 2.01653700 -1.72798100 0.08783700
H 1.77786100 -1.44805900 1.00863100
H 2.92251400 -1.32130200 -0.19182700
S -1.06886800 -0.43503700 -0.66931900
O -1.15611100 -0.88101600 0.72330700
O -2.23753400 -0.74954100 -1.43693300
O -0.93231700 1.13162700 -0.61759400
H -1.81402100 1.53295500 -0.31605100
O 0.18920500 -0.84926800 -1.29280600
H 1.23174000 -1.37207400 -0.53460600
O 1.48262800 1.66617600 0.84455400
H 1.36469800 1.04157200 1.57027700
H 0.68030300 1.59691300 0.30744700
O -3.21185000 1.98454600 0.21246100
H -3.76234000 2.41716700 -0.44348100
H -3.66571600 1.14058400 0.44232200
O -4.10628400 -0.52182800 0.67071900
H -3.78947500 -0.82266100 -0.19467300

H -3.41344100 -0.84357300 1.25805700
O 4.18868400 -0.71177000 -0.63528000
H 5.01116500 -1.01227100 -0.24530200
H 4.15910000 0.28068800 -0.55322200
O 3.90237200 1.84807100 -0.27578800
H 3.00431200 1.87105600 0.12569200
H 3.88960000 2.45899400 -1.01427100

$(H_2SO_4)(H_2O)_7$ [3-4] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 27.90, $\bar{\alpha}$ = 102.72

O 3.26298600 -1.54701000 -0.63276300
H 3.51540000 -2.34224300 -1.10538700
H 2.35842700 -1.30686900 -0.93229100
O 2.16879600 1.49190700 0.99299800
H 2.19879700 0.57724300 1.44832800
H 2.89104200 1.46274000 0.29667400
S -0.29787000 -0.02821800 -0.52038400
O 0.87546200 -0.55885000 -1.17195100
O -1.51529500 -0.07509500 -1.29597200
O -0.49940900 -0.93725500 0.73730000
H -1.42171700 -0.73352300 1.17662600
O -0.07020800 1.33722300 -0.00469700
H 1.20892600 1.51154400 0.52901900
O 2.12290500 -0.90152800 1.87457800
H 2.63571200 -1.38075400 1.20521800
H 1.19852100 -1.13867600 1.69772800
O -2.77076400 -0.41494200 1.66115900
H -2.93816800 0.51184900 1.42389700
H -3.35626400 -0.88695000 1.03588600
O -4.11020700 -1.14543300 -0.63284600
H -4.51544900 -0.27653300 -0.72610200
H -3.26828600 -1.05435200 -1.10020500
O 4.05109600 1.08420100 -0.73595300
H 3.98621800 0.11649700 -0.83675100
H 4.96454000 1.28982900 -0.52859700
O -3.36683600 1.68649200 -0.10444500
H -2.65509900 1.30925000 -0.64652100
H -3.22489100 2.63476000 -0.11064900

$(H_2SO_4)(H_2O)_8$ [0-8] Cluster (11.79 kcal/mol), $\Delta\alpha$ = 17.88, $\bar{\alpha}$ = 111.98

O -0.34069700 2.51132600 0.96967200
H -0.85059300 2.76405400 0.19034200
H 0.56181300 2.37598600 0.65544600
O -0.47891300 0.30657200 -1.39177600
H -0.36830200 -0.72907000 -1.49445500
H -1.31525600 0.42475700 -0.82549800
S 2.41979300 -0.15659300 0.15772900
O 1.50468500 -1.20229000 0.57207000
O 3.44202000 0.23082800 1.06748200
O 3.12510700 -0.80475600 -1.11576800
H 3.96597500 -0.35673100 -1.26587400
O 1.66501200 1.00083400 -0.38120500
H 0.40666700 0.64332800 -0.92324100
O -0.21991300 -2.17340500 -1.38541500

H 0.43136400 -2.20974600 -0.66407000
H -1.07060900 -2.48800800 -1.03587800
O -2.77919300 0.43141100 -0.31940800
H -2.93839100 0.11610700 0.62423200
H -3.10433800 1.33046100 -0.42653700
O -2.90129000 -2.35885200 -0.59336100
H -3.13968000 -1.43672700 -0.77064700
H -3.53346600 -2.90141600 -1.06891000
O -3.03273600 -0.69759900 1.96840900
H -2.08785700 -0.55244800 2.22187800
H -3.10307300 -1.62181700 1.71186600
O -1.84566800 2.84177000 -1.53041200
H -1.91233400 3.69326500 -1.96807700
H -1.34330100 2.27120100 -2.12252000
O -0.51774500 0.00899600 2.25472800
H -0.48532500 0.90480000 1.87841600
H 0.20466700 -0.48118800 1.83973200

$(H_2SO_4)(H_2O)_8$ [1-7] Cluster (3.17 kcal/mol), $\Delta\alpha$ = 23.68, $\bar{\alpha}$ = 111.95

O 1.60105700 -1.32769200 1.22167400
H 0.67898800 -1.45124200 1.48703100
H 1.93096600 -0.55783400 1.71639300
O 0.84778800 -0.76204500 -1.32707400
H 1.16928700 0.10031600 -1.65273400
H 1.19928300 -0.86956800 -0.41469400
S -2.11245100 -0.70176800 0.18785900
O -1.20635900 -1.18690100 1.17774600
O -3.49048300 -1.06019100 0.26033500
O -2.01796100 0.86583300 0.26863400
H -2.87793400 1.26409900 -0.04905400
O -1.60511700 -1.03023200 -1.20719000
H -0.55547400 -0.91142100 -1.28770100
O 0.59656800 2.15970100 0.59924600
H 0.94144700 2.16923200 -0.30732700
H -0.27088400 1.73975900 0.55881100
O 3.89901500 0.69654000 -0.36775700
H 3.65765900 0.85884500 0.55615100
H 3.92589500 -0.27201400 -0.47670700
O -4.43435400 1.44466500 -0.52978500
H -4.67417700 0.52373900 -0.35050800
H -5.04482700 1.99089700 -0.03042300
O 1.96645600 1.68954500 -1.79182100
H 2.79585700 1.38794900 -1.32606000
H 2.22195600 2.17895700 -2.57473000
O 2.52697500 1.11762800 2.07649700
H 2.70630400 1.55327400 2.91057500
H 1.77899900 1.59056400 1.63849600
O 3.59139500 -2.07133000 -0.64230400
H 3.03148100 -2.18903800 -1.41471100
H 2.98456000 -2.16239300 0.10584700

$(H_2SO_4)(H_2O)_8$ [2-6] Cluster (0.78 kcal/mol), $\Delta\alpha$ = 27.86, $\bar{\alpha}$ = 112.02

O -2.16409900 2.37931000 -0.22026500

H -2.31971600 3.30626200 -0.40976400
H -1.19856200 2.27680300 -0.09738500
O -0.97668400 -1.09978600 -1.39405800
H -1.10202800 -1.48000700 -0.48099800
H -1.84782300 -0.53281500 -1.57668100
S 1.34307100 0.85178200 0.00657800
O 0.38245900 1.82057700 0.50135800
O 2.71477300 1.26051500 0.11184800
O 1.10778100 -0.39398400 0.93970500
H 1.66353400 -1.15633200 0.58232800
O 1.01103500 0.36875800 -1.34765300
H -0.13629000 -0.46764400 -1.39529200
O -1.68008800 -1.87625000 1.01398900
H -1.63537300 -0.98553600 1.46616800
H -1.15013200 -2.48312500 1.53545200
O 2.54651800 -2.18322800 -0.25646800
H 2.28376500 -2.03448800 -1.16995800
H 3.44365400 -1.78957500 -0.18581400
O 4.71735000 -0.63264500 0.07458100
H 5.43517500 -0.43792600 -0.52920300
H 4.15592300 0.16291600 0.10088100
O -3.05237900 0.22720000 -1.64096400
H -2.85274400 1.08368400 -1.21423800
H -3.67856800 -0.23961500 -1.05605100
O -4.29918200 -1.30663700 0.25011500
H -3.53467100 -1.77471100 0.61869100
H -5.01861800 -1.93724100 0.19842100
O -1.66814600 0.53771600 1.99097400
H -2.30178300 1.11477900 1.54846100
H -0.80958200 0.93369100 1.77444100

$(H_2SO_4)(H_2O)_8$ [3-5] Cluster (3.15 kcal/mol), $\Delta\alpha$ = 27.06, $\bar{\alpha}$ = 112.10

O 2.96509800 -2.01026600 -0.92149400
H 3.50430700 -1.21988900 -1.06151600
H 2.11766100 -1.79837700 -1.33135200
O 1.86497400 1.99650500 -0.27418900
H 2.23058300 1.78621600 0.60482900
H 2.50130100 1.58986200 -0.88044900
S -0.70199100 -0.16554000 -0.68029300
O 0.38918300 -0.81145300 -1.32932400
O -2.02921800 -0.38339000 -1.18873800
O -0.65979300 -0.57244900 0.80304500
H -1.55317900 -0.28367800 1.30885300
O -0.50194300 1.35366900 -0.67439700
H 0.49492200 1.61671100 -0.49974700
O 2.06816800 -1.39959300 1.58828900
H 2.40588200 -1.76416600 0.74295400
H 1.12348100 -1.26616500 1.44595300
O -2.78570800 0.08160300 1.87244000
H -3.06265300 0.91421400 1.45697200
H -3.42896100 -0.55609900 1.49311300
O -4.42982600 -1.29922100 0.19708900
H -4.88123600 -0.49708200 -0.08869700

H -3.71592800 -1.40031000 -0.44569900
O 4.24552100 0.56042300 -0.81425000
H 5.11686000 0.80795200 -1.12795300
H 4.24295900 0.67035600 0.15306300
O -3.84586200 1.55972300 -0.25085000
H -3.19121700 1.09394600 -0.79406300
H -3.89174800 2.45381300 -0.59434000
O 3.31406600 0.85699900 1.75177100
H 2.83475600 -0.02349400 1.79459000
H 3.62678400 1.06443700 2.63305500

$(H_2SO_4)(H_2O)_8$ [4-4] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 17.88, $\bar{\alpha}$ = 110.55

O -1.79847600 1.44837400 1.47178200
H -1.11420700 0.81648100 1.19652900
H -2.21849600 1.02284500 2.22522200
O -2.82910100 -1.61989300 -0.41274600
H -2.77185200 -1.67160900 0.55470000
H -3.15596300 -0.71290800 -0.61956500
S 0.23487500 -0.48645800 -0.81881300
O -0.47014400 0.64934100 -1.37919000
O 1.60660600 -0.60288000 -1.27094800
O 0.18753200 -0.42438200 0.67839500
H 1.58172100 -0.10221500 1.32738800
O -0.48428900 -1.77271700 -1.21703100
H -1.49711200 -1.74038100 -0.91563600
O -1.88824000 -1.47066100 2.23069200
H -1.79225300 -2.21186900 2.83156800
H -1.02630600 -1.34299000 1.80405500
O 2.52971500 0.20314300 1.50508300
H 2.59993900 1.03560600 0.81903000
H 3.09568800 -0.53795800 1.13219500
O 0.08269300 3.03374200 -0.01167100
H -0.46627800 2.97790500 0.77931400
H -0.28203400 2.35037000 -0.59694100
O -3.30775000 0.98286600 -0.92883500
H -2.95535300 1.32734200 -0.09326300
H -2.55208400 1.05008500 -1.52460700
O 3.54122600 -1.78464100 0.22757500
H 4.40786600 -1.97036100 -0.13710300
H 2.93510800 -1.61012100 -0.51582900
O 2.50742700 1.99727300 -0.16269200
H 2.37546700 1.48299900 -0.97167100
H 1.66055500 2.50360400 -0.03769600

$(H_2SO_4)(H_2O)_9$ [0-9] Cluster (1.78 kcal/mol), $\Delta\alpha$ = 14.85, $\bar{\alpha}$ = 121.99

O 0.85517900 1.86266200 0.19671100
H 0.54153200 1.57860300 1.08334200
H 0.11734000 1.64237100 -0.39105300
O -0.93027600 -2.55213900 0.12227200
H -0.40126400 -2.27527500 -0.74181000
H -0.35628000 -2.38473800 0.92552200
S -2.46789000 0.46524500 -0.25508400
O -1.29284500 0.51732000 -1.10325700

O -2.47491200 1.40398600 0.83438600
O -3.63739700 0.88717900 -1.23668300
H -4.43742900 1.05313900 -0.72322000
O -2.78704800 -0.90002100 0.17233700
H -1.73911000 -1.90285500 0.16383300
O 0.15482600 -1.70082900 -1.93354400
H 1.12366400 -1.58151800 -1.96939800
H -0.25882600 -0.82121100 -1.91626100
O 2.97146600 -1.70163600 1.02380200
H 3.20889400 -0.77879000 0.82935100
H 3.02614400 -2.12353800 0.15763700
O 2.88646600 -1.44074100 -1.85279500
H 3.40050400 -1.55349600 -2.65404700
H 3.11612300 -0.56354500 -1.47445600
O 3.20089800 0.71057400 -0.31045500
H 2.28748900 1.05237300 -0.15328400
H 3.71879600 1.52587000 -0.34648300
O 0.61538600 -1.96534100 2.13065200
H 1.53569700 -1.86363200 1.76112600
H 0.67930300 -2.54134600 2.89555800
O 3.11111800 3.48655400 -0.28226800
H 3.27896200 4.30734700 0.18162500
H 2.20058900 3.23287200 -0.06839000
O -0.21785200 0.85145100 2.47167400
H -0.06586800 -0.10141800 2.48600500
H -1.13009400 0.98270900 2.17309200

$(H_2SO_4)(H_2O)_9$ [1-8] Cluster (1.48 kcal/mol), $\Delta\alpha$ = 28.39, $\bar{\alpha}$ = 121.88

O 1.24700400 -0.99780600 -0.91068300
H 1.09567300 -0.52010900 -0.06693800
H 0.55427900 -1.66984600 -0.91176600
O -0.32931000 1.04114700 -2.00829500
H 0.07709900 1.78225400 -1.51656400
H 0.25361000 0.28161100 -1.82436000
S -2.59639100 -0.69192900 -0.28056800
O -1.46567800 -1.54217500 -0.46270000
O -3.90286200 -1.25727500 -0.19912700
O -2.32220200 0.07952400 1.06405200
H -3.18920800 0.41508100 1.42713000
O -2.61406300 0.40425900 -1.33573200
H -1.63424200 0.70360400 -1.62491200
O 0.55534400 0.50288700 1.27597500
H -0.37620300 0.30820900 1.43861300
H 0.58654600 1.39907800 0.90123700
O 3.43195600 1.64170600 -0.25092600
H 3.70401700 0.93779700 -0.85364700
H 3.46629600 1.23337600 0.64440500
O -4.80468600 0.58382000 1.71541700
H -5.26210300 1.37671200 1.42733700
H -5.05685800 -0.11653500 1.09610800
O 3.28439700 0.36901000 2.12213100
H 3.70229500 -0.49103000 1.94895200
H 2.33284300 0.21337400 2.16135700

O 4.58872800 -1.89981600 1.13958800
H 4.51571800 -1.66156500 0.20153500
H 5.52524000 -1.97837700 1.32720600
O 3.88862300 -0.96166500 -1.41586800
H 4.14165500 -1.29207400 -2.27933200
H 2.92465500 -1.11211400 -1.32354100
O 1.07363200 2.69423300 -0.36201700
H 2.01511800 2.35246200 -0.39656900
H 1.11876400 3.64615300 -0.26168800

$(H_2SO_4)(H_2O)_9$ [2-7] Cluster (2.86 kcal/mol), $\Delta\alpha$ = 29.38, $\bar{\alpha}$ = 123.12

O -1.97171600 1.43145800 -0.27194600
H -2.39216400 0.56441500 -0.09312900
H -1.23864900 1.23002600 -0.87057600
O -0.95189400 -2.45265200 0.06598600
H -1.76163200 -2.03313900 -0.26302400
H -0.98042100 -2.26506000 1.02135600
S 1.53621700 -0.44486100 -1.09819500
O 0.36422500 0.33198200 -1.35588000
O 2.68662600 -0.26624600 -1.92098300
O 1.94310600 -0.13920900 0.37918700
H 2.96366600 -0.17652800 0.46560900
O 1.18497200 -1.92772800 -1.09071400
H 0.27840000 -2.12636600 -0.61104600
O -0.30176700 0.88480200 1.93563200
H -0.86867700 1.27694600 1.24984300
H 0.51533500 0.65198800 1.47629400
O 4.46889800 -0.22261400 0.29399800
H 4.48649000 -0.26576800 -0.67091200
H 4.94495900 0.58539200 0.54942000
O 5.78654200 2.10361000 1.07607600
H 6.40648600 2.07840700 1.80785700
H 5.28798000 2.91713700 1.17775800
O -3.23672600 -0.91074300 0.33474600
H -3.08817800 -1.07023900 1.27655000
H -4.17004800 -0.64441600 0.20058900
O -1.55319500 -1.37255000 2.52903400
H -1.06764600 -0.51603800 2.42189700
H -1.47506500 -1.63548700 3.44672400
O -4.39912100 2.55079000 -0.87534700
H -3.46465000 2.30309500 -0.73780400
H -4.53525800 3.36188500 -0.38375900
O -5.63628400 0.22215500 -0.17013200
H -5.30509500 1.10374300 -0.43688300
H -6.18462600 -0.08665300 -0.89290000

$(H_2SO_4)(H_2O)_9$ [3-6] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 34.91, $\bar{\alpha}$ = 122.10

O -2.75604000 -1.12709000 -0.65472800
H -3.69674300 -1.38756400 -0.58381400
H -2.19722900 -1.89988400 -0.78179200
O -1.60098100 0.24817300 1.36285900
H -1.73062900 1.17001400 1.08248000
H -2.06979300 -0.28648700 0.67951000

S 1.06901200 -0.94293600 -0.19897600
O -0.04041900 -1.62833100 -0.77443100
O 2.34364300 -1.59450100 -0.17466400
O 1.19030100 0.40010000 -0.95927500
H 1.97617900 0.96065400 -0.57295500
O 0.76452700 -0.52331100 1.24576800
H -0.21930600 -0.17343100 1.33301900
O -1.53258400 1.04422200 -1.93541300
H -1.96902400 0.20542500 -1.71434100
H -0.59040700 0.86935100 -1.82153900
O 3.07308100 1.66681700 0.10202000
H 3.24609100 1.20108800 0.93308900
H 3.92221000 1.57481800 -0.37190700
O 5.54164500 0.81527900 -0.68825400
H 6.40683700 1.22258400 -0.63047800
H 5.46248900 0.21273600 0.06681800
O -4.60003300 0.96521400 1.24261600
H -4.03195100 0.64144900 1.94739600
H -4.03535800 1.57523200 0.74194300
O 4.30534400 -0.53075000 1.42035400
H 4.44888700 -0.99788200 2.24469600
H 3.65300300 -1.05333000 0.91771100
O -2.53534000 2.47850600 0.02613600
H -2.15683200 2.07346400 -0.79639100
H -2.43450200 3.42876100 -0.04123900
O -5.36839400 -1.29234700 -0.10211100
H -5.25962100 -0.44208800 0.36733700
H -6.10649400 -1.18379200 -0.70293400

$(H_2SO_4)(H_2O)_9$ [4-5] Cluster (0.52 kcal/mol), $\Delta\alpha$ = 36.06, $\bar{\alpha}$ = 121.88

O 3.40770100 -1.59304900 -0.03949000
H 2.83640900 -2.35401300 -0.17470600
H 2.99184900 -1.08403600 0.69346800
O 2.35071000 0.40407300 -1.64877900
H 2.79998000 1.13896100 -1.19728200
H 2.72637100 -0.39833100 -1.23425800
S -0.45672800 -0.69300700 -0.27339200
O 0.54288200 -1.69304700 -0.10680400
O -1.82290800 -1.08558200 -0.46034500
O -0.38118300 0.20795300 0.99514200
H -1.16780300 0.86529300 1.01480500
O -0.10252600 0.24291100 -1.42525000
H 0.94643300 0.35073000 -1.52925800
O 2.46172000 0.18758900 1.74400100
H 2.79499700 1.00964600 1.35923500
H 1.49947500 0.23230500 1.68752600
O -2.41963000 1.70938500 0.97279800
H -2.88935600 1.55545300 0.08819300
H -2.31333200 2.65588500 1.08618200
O -3.89513200 -0.75989900 1.53650300
H -3.21798400 -1.13472000 0.95641700
H -3.53504900 0.10045400 1.77832500
O 5.67387400 -0.06572600 0.11331100

H 6.15156100 -0.25569000 0.92300600
H 5.06530500 -0.81335400 -0.01349000
O -3.55468700 1.14099100 -1.25611200
H -3.03196500 0.37112900 -1.51343500
H -4.44724500 0.78953300 -1.06678300
O -5.77826800 -0.13300400 -0.34490400
H -5.27322500 -0.43771900 0.43378700
H -6.64801300 0.12326600 -0.03772100
O 3.90370500 1.96211000 0.05354200
H 4.65840700 1.33251600 0.08506800
H 4.27076300 2.84314900 -0.03371300

$(H_2SO_4)(H_2O)_{10}$ [0-10] Cluster (2.75 kcal/mol), $\Delta\alpha$ = 15.27, $\bar{\alpha}$ = 131.64

O -0.77887300 1.35270400 1.82307500
H -1.70969400 1.05549700 2.11117600
H -0.83875700 1.91892500 0.90190500
O 0.47429500 -0.83336100 1.25290100
H 0.93806900 -0.73464100 0.39092700
H -0.23606900 0.52269600 1.62785100
S -2.41736900 -0.66317900 -0.69721800
O -1.31858500 -0.00302000 -1.37917000
O -3.46993600 0.24159000 -0.28410500
O -3.02626300 -1.58012800 -1.84071100
H -3.82950600 -2.00351200 -1.51492100
O -1.99299800 -1.55396600 0.36993300
H -0.33840900 -1.32446700 1.01787900
O 1.36665200 -0.64474500 -1.29536000
H 0.46395800 -0.45504400 -1.59960700
H 1.92738500 0.12615400 -1.48494300
O 4.19788000 -0.38959400 0.50379700
H 3.80525300 -0.52895600 1.38190500
H 4.07401000 -1.22991700 0.02922700
O 3.31014000 1.33571200 -1.21467300
H 3.68571100 0.75266800 -0.49212200
H 3.98998400 1.40754100 -1.88747700
O 1.54383700 3.39655900 -0.97605800
H 2.24722200 2.72000600 -1.00245100
H 1.91651400 4.17215500 -0.55492800
O 2.78578900 -1.07422600 2.80899900
H 1.88662100 -1.09239600 2.44613300
H 2.73122500 -0.62257800 3.65218100
O -0.90101000 2.54306000 -0.30526500
H -1.16032700 1.84355600 -0.92816600
H -0.02377300 2.88910700 -0.58853800
O -3.13489000 0.53248400 2.38491800
H -3.45892100 0.46396400 1.46199600
H -3.10527500 -0.37826900 2.69147900
O 3.43103700 -2.49994400 -1.13851900
H 2.57654400 -2.08115300 -1.32585700
H 3.23954400 -3.39546600 -0.85626200

$(H_2SO_4)(H_2O)_{10}$ [1-9] Cluster (4.46 kcal/mol), $\Delta\alpha$ = 24.19, $\bar{\alpha}$ = 131.89

O 1.47824700 0.39474500 -1.52533500

H 0.54362100 0.15051800 -1.62472200
H 1.97811200 -0.41801500 -1.68438800
O -0.40503500 1.86003200 1.46052000
H -0.35108700 0.97941600 1.99340700
H 0.52181200 2.14614400 1.22317300
S -2.15734300 0.04200200 -0.78365200
O -1.09583300 -0.71122400 -1.42393900
O -3.45348700 -0.07911600 -1.38510500
O -2.25617100 -0.60024500 0.66990500
H -3.21294300 -0.69570000 0.91937400
O -1.75598500 1.43421400 -0.54855500
H -0.98163500 1.69953300 0.58819500
O 0.67259200 -2.12778800 0.21579700
H -0.05384900 -1.74159800 -0.30127700
H 1.15033600 -1.37338100 0.60211300
O 2.33175500 -0.32099100 1.59657200
H 3.15350000 -0.78422200 1.34590000
H 2.40519100 0.58345800 1.26035700
O -4.89213500 -0.72390400 0.86634100
H -4.85510100 -0.47489700 -0.07118600
H -5.34044300 -1.57105000 0.90254700
O 4.44069900 -1.69912200 0.51971900
H 4.81096600 -2.47770600 0.93849000
H 3.97590100 -2.01174000 -0.27580400
O 2.66102300 -2.25757700 -1.52235700
H 2.61952500 -2.88132100 -2.24888400
H 1.87536700 -2.41716300 -0.94319500
O 2.39391000 2.86765500 -1.60917800
H 3.22272400 2.97465800 -2.07773600
H 2.07120100 1.95744100 -1.79646700
O -0.18387100 -0.33890600 2.68542400
H 0.75210100 -0.56410000 2.54515100
H -0.69348600 -0.95697700 2.14502000
O 2.08513600 2.47086800 0.94943000
H 2.47498300 3.15052800 1.50264800
H 2.28393100 2.70499400 0.00178700

$(H_2SO_4)(H_2O)_{10}$ [2-8] Cluster (3.74 kcal/mol), $\Delta\alpha = 31.42$, $\bar{\alpha} = 132.27$

O 1.83260600 1.47501100 -0.06770200
H 0.86087800 1.48887800 -0.12146600
H 2.10831900 0.73040500 -0.62868900
O 0.11429000 -1.01091300 1.78774800
H 0.42173700 -1.17272000 0.86014500
H 0.84111900 -0.52800800 2.21216600
S -2.09926500 0.75028200 0.08607400
O -0.93143900 1.51585500 -0.21843600
O -3.36705700 1.39659100 -0.04514600
O -2.04536200 -0.49093000 -0.84602600
H -2.85915900 -1.09745300 -0.68706800
O -2.02317800 0.16491100 1.49067700
H -1.08595600 -0.31766200 1.66866100
O 0.80469800 -1.14745300 -0.75568200
H 1.43995300 -1.78516900 -1.14326800

H -0.00829300 -1.14057900 -1.27012900
O -4.10924000 -1.90255600 -0.46282400
H -4.85179800 -1.25480100 -0.49649700
H -4.14869900 -2.32166300 0.40001400
O -5.80035600 0.15215000 -0.47591700
H -5.07247400 0.77619700 -0.31577200
H -6.24981800 0.45810700 -1.26539800
O 4.08052900 -1.59741100 1.00354800
H 3.56033100 -0.99615300 1.56636600
H 4.76781900 -1.96814300 1.55944700
O 2.94418500 -2.59796300 -1.51051500
H 3.36486200 -1.82821700 -1.91718300
H 3.31424800 -2.59256500 -0.61762900
O 3.92095200 0.01472600 -1.31794300
H 4.28172400 -0.36030400 -0.50338700
H 4.24577800 0.92644700 -1.37312400
O 2.50767200 0.35618400 2.23041800
H 2.29129600 0.88619700 1.42046900
H 2.82596000 0.97145900 2.89355000
O 4.10606700 2.79335200 -0.97673000
H 4.07103600 3.49920700 -1.62370500
H 3.19443300 2.64958600 -0.67844000

$(H_2SO_4)(H_2O)_{10}$ [3-7] Cluster (5.01 kcal/mol), $\Delta\alpha$ = 35.66, $\bar{\alpha}$ = 132.05

O -2.07920000 -1.45025800 -0.05515600
H -2.99606300 -1.75854100 0.12817200
H -1.50052100 -2.19491800 -0.24137100
O -0.75129400 0.21581600 1.58760000
H -1.13573200 1.07017600 1.33474200
H -1.26211100 -0.45275800 1.07303000
S 1.73159400 -0.70465300 -0.41232600
O 0.61443200 -1.55465200 -0.66271100
O 3.05268900 -1.23030600 -0.53339800
O 1.57727800 0.50051500 -1.37327900
H 2.38302300 1.15130800 -1.28738700
O 1.61377300 -0.08503200 0.98969400
H 0.59125200 0.07313700 1.26181700
O -1.35761100 0.70916400 -1.66603800
H -1.61329800 -0.16112800 -1.31425200
H -0.39930500 0.66563200 -1.77184800
O 3.56181900 1.98886000 -1.04291200
H 3.91148200 1.73250200 -0.14053900
H 3.43772300 2.93967300 -1.04065500
O 5.55310000 -1.19359200 0.72886100
H 4.76164000 -1.42011900 0.21823100
H 6.29392700 -1.29496200 0.12943400
O -4.62582900 1.06699800 1.14748000
H -4.85164900 1.49092100 1.97706100
H -3.80011700 1.48920900 0.83993000
O 4.28340900 1.16985100 1.32124100
H 3.45910000 0.76603500 1.61792800
H 4.89381900 0.41713900 1.20371100
O -2.24592700 2.18312500 0.28118700

H -1.90992500 1.71544300 -0.53658500
H -2.21585000 3.12402400 0.10028200
O -6.19708800 -0.06694000 -0.93590600
H -7.10749700 0.19601500 -1.07437600
H -5.82875000 0.54574300 -0.28361900
O -4.61862000 -1.78632300 0.63530000
H -5.24917900 -1.61645500 -0.07836900
H -4.61492100 -0.94141800 1.10617900

$(H_2SO_4)(H_2O)_{10}$ [4-6] Cluster (0.00 kcal/mol), $\Delta\alpha$ = 33.69, $\bar{\alpha}$ = 130.94

O 3.13674900 -2.10756200 -0.45999200
H 3.48193900 -3.00181600 -0.48525100
H 2.19489700 -2.16611400 -0.70962400
O 1.92216200 1.24527000 -0.50347500
H 1.97644800 0.77481700 0.35256800
H 2.81870900 1.06673800 -0.89311700
S -0.57744800 -1.02875200 -0.52727100
O 0.43605400 -2.04252100 -0.65935700
O -1.90604900 -1.41888700 -0.94218800
O -0.57425700 -0.44831200 0.83998400
H -1.21623200 1.00500000 0.82753600
O -0.22471200 0.16292700 -1.47845200
H 0.66030400 0.55656700 -1.21075100
O 2.17199000 -0.49900600 1.64337000
H 2.55559000 -1.21312800 1.10754400
H 1.22062000 -0.67851800 1.67143000
O -1.68926900 1.86979400 0.61990400
H -2.44115500 1.57213600 -0.11801800
H -1.00531900 2.49258800 0.21912400
O -3.37499700 -1.43750400 1.48715500
H -3.01588100 -1.68857400 0.62256600
H -2.60052000 -1.10114300 1.94709400
O 4.34235700 0.41381000 -1.09422300
H 4.12633700 -0.52985900 -1.07033100
H 4.69959900 0.60012200 -0.21127000
O -3.33552800 1.05677300 -0.98039600
H -2.96384100 0.20513600 -1.26941300
H -4.16085100 0.83816700 -0.48215100
O -5.30988000 0.21993700 0.57694500
H -5.84408100 0.71210000 1.20110900
H -4.73146300 -0.37944100 1.09071600
O 4.66231600 0.76386100 1.68425700
H 3.79414400 0.46916000 1.99216900
H 4.94620700 1.45882300 2.27906000
O 0.20536900 3.34110000 -0.33418800
H 0.96166500 2.72925500 -0.44102000
H 0.08361300 3.78056600 -1.17838800

$(H_2SO_4)(H_2O)_{10}$ [5-5] Cluster (3.05 kcal/mol), $\Delta\alpha$ = 38.09, $\bar{\alpha}$ = 132.16

O 3.73495700 -1.06544000 -1.53421500
H 4.15276200 -1.74978700 -2.06021800
H 2.76735400 -1.21931600 -1.58447300
O 2.14095200 1.52098100 0.26153100

H 2.48479300 0.73154900 0.76364200
H 2.89565400 1.69475100 -0.42654200
S 0.03151000 -0.85739800 -0.47540200
O 1.14758300 -1.47557900 -1.14839200
O -1.26175300 -1.40119500 -0.76220900
O 0.34378000 -1.08488700 1.04870500
H -0.44160100 -0.76068200 1.62139400
O 0.03934800 0.62051600 -0.64730900
H 1.22882100 1.20224700 -0.18235000
O 3.18090400 -0.73016400 1.19936600
H 3.48949000 -1.07578400 0.34307200
H 2.35985400 -1.20570900 1.39292300
O -1.64903100 -0.21735400 2.37246200
H -2.42704500 -0.71347700 2.06203400
H -1.81331600 0.66977300 2.02081100
O -6.02296700 -0.34043100 -0.36726900
H -6.42311600 -0.67477400 -1.17101900
H -5.77909900 0.58821000 -0.55081700
O 4.17163500 1.66449200 -1.19514500
H 4.16717700 0.77089700 -1.57816200
H 4.81636900 1.61229400 -0.46870800
O -2.61000200 1.42219900 0.20572000
H -1.79152400 1.33107600 -0.30227600
H -2.97030600 0.51676300 0.25745600
O -5.06112800 2.20219900 -0.77112200
H -4.13392700 2.10273300 -0.48458800
H -5.42248500 2.92204000 -0.25189600
O 5.38986200 1.00084900 1.20975100
H 4.77346700 0.37043500 1.60402400
H 5.88804900 1.39137300 1.92893900
O -3.63352300 -1.13900900 0.67281100
H -4.53513300 -1.04500700 0.30968900
H -3.07531500 -1.55865000 0.00601500

$(H_2SO_4)(NH_3)(H_2O)$ [0-1] Cluster (2.21 kcal/mol), $\Delta\alpha = 13.72$, $\bar{\alpha} = 58.22$

S -0.90772900 -0.09419400 0.08880800
O 0.02751800 0.14933200 1.17088200
O -2.28755800 -0.22107500 0.41793700
O -0.77413000 1.25198600 -0.78769400
H -1.61926900 1.41055600 -1.22290600
O -0.39987900 -1.15975900 -0.79280600
H 1.02252400 -1.36260800 -0.47229300
N 2.05559200 -1.33763800 -0.08790400
H 2.01005600 -1.58962300 0.89596400
H 2.35073800 -0.34114300 -0.14671700
H 2.68623900 -1.95389000 -0.58711600
O 2.22459800 1.41194900 0.08674200
H 1.94560200 1.96871500 -0.64421600
H 1.41423000 1.27908800 0.61120600

$(H_2SO_4)(NH_3)(H_2O)$ [1-0] Cluster (0.00 kcal/mol), $\Delta\alpha = 20.44$, $\bar{\alpha} = 58.81$

S 0.02917100 0.43961800 -0.02590500
O -0.98608600 1.27473700 0.52063600

O 1.09187200 1.00801300 -0.79283000
O 0.65097400 -0.34284800 1.17114800
H 1.54870200 -0.67384000 0.90943700
O -0.62270300 -0.66135900 -0.88322200
H -1.60478600 -0.80842200 -0.57753200
N -3.07057400 -0.78172100 -0.01247000
H -3.80949800 -0.74359200 -0.70357000
H -3.03955100 0.11139100 0.47200400
H -3.30688800 -1.49927300 0.66167800
O 3.02494000 -0.81226200 0.07679200
H 3.19093200 -1.58097400 -0.47252500
H 2.77639700 -0.09737500 -0.52791300

$(H_2SO_4)(NH_3)(H_2O)_2$ [0-2] Cluster (2.82 kcal/mol), $\Delta\alpha = 16.32$, $\bar{\alpha} = 67.81$

S 1.28459600 0.08990600 0.02405600
O 0.35532300 -0.04860800 1.13581000
O 2.67375400 0.12576100 0.34351800
O 1.06246600 -1.28334800 -0.79573300
H 1.91647800 -1.54753000 -1.15547400
O 0.83793300 1.14637200 -0.88737300
H -0.51460500 1.69833800 -0.36280500
N -1.39582400 1.91194600 0.21555800
H -1.67842100 2.88286400 0.14763600
H -1.12628300 1.67609600 1.17032000
H -2.16823400 1.26465200 -0.07268700
O -1.54732200 -1.94078100 0.39735600
H -0.89568800 -1.39608800 0.87322200
H -1.02172800 -2.31097900 -0.31766200
O -3.23945600 -0.00889000 -0.31355700
H -3.73379200 -0.20194700 -1.11117300
H -2.70208900 -0.81158100 -0.10533500

$(H_2SO_4)(NH_3)(H_2O)_2$ [1-1] Cluster (2.15 kcal/mol), $\Delta\alpha = 21.95$, $\bar{\alpha} = 68.07$

S -0.32850500 -0.43337000 0.23164600
O 0.67243900 -0.16081600 1.24585600
O -1.55216400 -1.03267600 0.68743900
O -0.69903800 1.00166600 -0.33280400
H -1.66703400 1.04038300 -0.52209900
O 0.27813400 -1.15190400 -0.90215000
H 1.73150300 -1.00479900 -0.79376000
N 2.77380200 -0.74676500 -0.53195800
H 3.45389400 -1.06312300 -1.21308800
H 2.95883200 -1.15575100 0.38011800
H 2.77810900 0.28836500 -0.42260900
O 2.20485400 1.87371300 0.14897500
H 1.61380000 2.35047900 -0.44006100
H 1.59997700 1.42954800 0.76906300
O -3.34923400 0.63400000 -0.55758000
H -3.95309000 1.12927500 -0.00128900
H -3.11645800 -0.16495900 -0.05680300

$(H_2SO_4)(NH_3)(H_2O)_2$ [2-0] Cluster (0.00 kcal/mol), $\Delta\alpha = 23.21$, $\bar{\alpha} = 68.92$

S 0.40063700 -0.49094600 0.19687700

O 1.51662000 -1.15796800 0.77844200
O -0.71581300 -1.26782300 -0.24729300
O -0.07755000 0.56046400 1.22094900
H -0.90684800 1.04529100 0.88460800
O 0.87017000 0.35044300 -1.00975400
H 1.87055100 0.59365600 -0.89051200
N 3.40338900 0.73230600 -0.53097600
H 4.05247800 0.50097100 -1.27276300
H 3.45627300 0.00493000 0.17745900
H 3.70156200 1.60470900 -0.11251600
O -2.17599900 1.70953300 0.31673200
H -2.73714100 0.98270800 -0.03847200
H -2.00376900 2.30084800 -0.41917100
O -3.32292900 -0.48686300 -0.67881300
H -3.95332200 -1.01740500 -0.18894300
H -2.46968100 -0.94900300 -0.61500200

$(H_2SO_4)(NH_3)(H_2O)_3$ [0-3] Cluster (2.27 kcal/mol), $\Delta\alpha = 13.27$, $\bar{\alpha} = 76.56$

S 1.43386000 0.10339100 -0.05804900
O 0.85058400 0.83921200 1.07119400
O 2.82150700 0.34747800 -0.27361000
O 1.29822000 -1.44421800 0.35159000
H 2.12076500 -1.71950800 0.77255900
O 0.56427700 0.19345000 -1.22316200
H -0.67574300 2.12068200 -1.15140400
N -1.10281400 2.17322700 -0.22798300
H -0.37459700 1.79095000 0.42764100
H -1.94550800 1.50861900 -0.20329100
H -1.36481300 3.12478800 0.00359900
O -1.41639600 -0.93130300 1.69098100
H -1.21557800 -1.54497800 0.97206500
H -0.59934000 -0.42569700 1.79687400
O -1.50654500 -1.62811600 -1.19844800
H -1.38915100 -2.41221300 -1.73655300
H -0.70647300 -1.08529600 -1.32508700
O -3.05090100 0.38677400 -0.04971900
H -2.68112000 -0.04774000 0.74651500
H -2.87646900 -0.28267600 -0.72886900

$(H_2SO_4)(NH_3)(H_2O)_3$ [1-2] Cluster (0.00 kcal/mol), $\Delta\alpha = 17.31$, $\bar{\alpha} = 77.08$

S 0.81707800 -0.21269300 -0.47209000
O -0.35299100 -0.13195200 -1.32923900
O 2.07829600 -0.37890500 -1.13256100
O 0.84349400 1.21095000 0.23922900
H 1.66984200 1.24182800 0.77021200
O 0.61071600 -1.18202400 0.61735200
H -0.86561700 -1.69769400 0.50621000
N -1.86812000 -1.89662800 0.18162700
H -2.50722900 -1.15036100 0.54914000
H -2.18594700 -2.82277300 0.44293400
H -1.82624100 -1.79591000 -0.83209700
O -1.89227800 2.00835800 -0.41334800
H -1.42479100 1.37305900 -0.98217800

H -1.17430800 2.35953100 0.12242900
O -3.41375000 0.22487000 0.83300800
H -3.82180100 0.54645900 1.63745700
H -2.91074500 0.97921800 0.43599900
O 3.22266500 0.47401400 1.35422800
H 2.88392200 -0.29695600 1.81992600
H 3.39727500 0.14057800 0.46266500

$(H_2SO_4)(NH_3)(H_2O)_3$ [2-1] Cluster (1.18 kcal/mol), $\Delta\alpha = 20.27$, $\bar{\alpha} = 77.56$

S 0.00662800 -0.58496300 -0.09006100
O -1.20693300 -1.20835900 -0.57873600
O 1.20022100 -1.37732900 -0.19635200
O 0.17056000 0.68822600 -0.99914300
H 0.90013500 1.24905900 -0.59800400
O -0.18635500 -0.05217700 1.28021400
H -1.67283700 0.05969800 1.47394900
N -2.76237400 0.05068700 1.38037000
H -2.97365000 0.52336200 0.47252300
H -3.23785300 0.48827200 2.16103900
H -3.04038800 -0.92319600 1.28932400
O 2.02427800 1.85894800 0.41270700
H 1.63419300 1.56792200 1.24423400
H 2.79047300 1.26624500 0.27600400
O 3.70323800 -0.20425600 -0.15887400
H 4.32613900 -0.66949400 0.40057100
H 2.91427300 -0.77175500 -0.21879100
O -2.91591600 0.85832000 -1.23670500
H -2.32153300 0.09749400 -1.36592300
H -2.40114400 1.60999900 -1.54142700

$(H_2SO_4)(NH_3)(H_2O)_3$ [3-0] Cluster (0.42 kcal/mol), $\Delta\alpha = 23.83$, $\bar{\alpha} = 78.50$

S 0.52803900 -0.63272000 -0.10397700
O 1.57606200 -1.59638600 -0.02689900
O -0.54953800 -0.84121800 -1.02406700
O -0.02480800 -0.41027600 1.29971300
H -0.96251700 0.10402700 1.28679100
O 1.15635900 0.74141900 -0.49370600
H 2.16117600 0.75616500 -0.22164500
N 3.64918500 0.49438300 0.18544700
H 4.35037100 0.71586100 -0.51055500
H 3.59749100 -0.51724300 0.27678100
H 3.95327800 0.87707900 1.07227900
O -2.18330400 0.77653200 1.18461200
H -2.77099300 0.15813900 0.70476400
H -1.99816200 1.51262700 0.57061900
O -3.26175500 -1.13202900 -0.41806100
H -3.52259500 -2.00686900 -0.12628700
H -2.36884400 -1.22404800 -0.78651400
O -1.12289800 2.55978600 -0.61506100
H -0.31171900 2.06482300 -0.79418000
H -0.84134800 3.43965500 -0.35878800

$(H_2SO_4)(NH_3)(H_2O)_4$ [0-4] Cluster (6.88 kcal/mol), $\Delta\alpha = 14.32$, $\bar{\alpha} = 87.42$

S -1.73231200 -0.18858900 -0.21231900
O -0.51690400 -0.14642400 -0.99684900
O -2.94035500 -0.55749400 -0.84660600
O -1.51239900 -1.19216200 0.95571900
H -0.61928100 -1.04889700 1.36231400
O -1.86792500 1.16108100 0.49314400
H -1.09750900 1.83970600 0.17658000
N -0.00093800 2.66590900 -0.35037300
H 0.87207600 2.34501300 0.06688200
H -0.07299700 3.67063400 -0.25199500
H 0.03520800 2.43549600 -1.33751800
O 1.51980300 -2.04090400 -0.75263500
H 1.45346000 -2.17730700 0.19839500
H 0.72921600 -1.51770800 -0.96780600
O 0.94860700 -0.87705000 1.89105700
H 1.07472600 -0.89944000 2.84170600
H 1.43760200 -0.09568100 1.55594800
O 2.37456000 1.20735000 0.82111900
H 3.08593200 1.56704600 1.35489200
H 2.81404000 0.74966300 0.05727600
O 3.45151600 -0.24457300 -1.08344300
H 3.55665300 -0.00500600 -2.00509800
H 2.79920100 -0.98605600 -1.05390700

$(H_2SO_4)(NH_3)(H_2O)_4$ [1-3] Cluster (0.00 kcal/mol), $\Delta\alpha = 14.68$, $\bar{\alpha} = 86.81$

S 0.82933300 -0.58244000 -0.07566700
O 0.27458400 -1.83015700 0.37756000
O 1.24177500 0.31961600 1.00838700
O 2.13484800 -0.95812800 -0.84887700
H 2.79184900 -0.22709000 -0.77507900
O -0.04733500 0.11968100 -1.01277800
H -1.59933100 1.73631900 0.85567600
N -1.32096900 1.17973000 1.69455800
H -0.29788600 1.01613000 1.64005100
H -1.78664500 0.22846400 1.60939900
H -1.57794700 1.64555100 2.55702400
O -2.65520800 -0.40953200 -1.45861200
H -1.67636400 -0.39672000 -1.43151400
H -2.90375700 -0.89390400 -2.24786600
O -1.84886200 2.27275500 -0.78550200
H -1.01290400 1.89113500 -1.09252200
H -2.50028300 1.65754400 -1.14934200
O 3.64181000 1.14559300 -0.10137200
H 2.96528900 1.15147600 0.59343300
H 4.47591600 0.95914500 0.33366600
O -2.32789900 -1.26482000 1.20906700
H -2.72549700 -1.15267000 0.33164000
H -1.48470100 -1.71451400 1.02122400

$(H_2SO_4)(NH_3)(H_2O)_4$ [2-2] Cluster (0.61 kcal/mol), $\Delta\alpha = 19.76$, $\bar{\alpha} = 86.85$

S 0.33465200 -0.57220200 -0.42784500
O -0.97803500 -0.94919700 -0.90571000
O 1.44243500 -1.27716700 -1.00808000

O 0.44188200 0.94412500 -0.86556600
H 1.34812400 1.30454400 -0.61361700
O 0.39780900 -0.55229400 1.04678800
H -0.95764500 0.02907000 1.62225500
N -1.91328400 0.47407600 1.80419300
H -1.96756700 0.89303800 2.72510400
H -2.64473000 -0.22806200 1.66281100
H -2.06161300 1.17851800 1.03953300
O 3.32791500 -0.69739700 1.00540300
H 2.57626400 -0.73819800 1.60810600
H 2.97812900 -1.16402100 0.23044600
O 2.79652400 1.70989500 -0.09176000
H 3.43188900 1.91828900 -0.77941000
H 3.12452500 0.89192400 0.34999500
O -2.27491600 1.84924600 -0.51716700
H -2.84696700 1.16808900 -0.89080400
H -1.40363900 1.68837400 -0.90991000
O -3.50336000 -0.84251400 -0.04619900
H -2.62978400 -1.05992300 -0.42888800
H -4.11047200 -1.52249800 -0.34112000

$(H_2SO_4)(NH_3)(H_2O)_4$ [3-1] Cluster (1.73 kcal/mol), $\Delta\alpha$ = 22.03, $\bar{\alpha}$ = 86.97

S 0.31644400 -0.25602200 -0.60335600
O 1.58406000 -0.63032900 -1.19597500
O -0.85368700 -0.53548500 -1.39414100
O 0.24030500 -1.09960500 0.70685100
H -0.66678600 -0.96305700 1.16487300
O 0.34976200 1.16493300 -0.17186400
H 1.82720800 1.53579800 -0.02729500
N 2.91112000 1.53337800 -0.00051500
H 3.30340600 2.37161000 0.41274300
H 3.22889700 1.41993600 -0.95979500
H 3.17755000 0.66701500 0.52542300
O -2.03046900 -0.64930700 1.76358800
H -2.70700400 -0.99897100 1.16672700
H -2.13088400 0.31735300 1.64157100
O -3.47111700 -0.43386400 -0.65475500
H -4.09763700 -0.75705900 -1.30357300
H -2.58459000 -0.53074000 -1.05022300
O 3.25519500 -0.99124400 0.99024800
H 2.68746400 -1.24439300 1.72377600
H 2.74052300 -1.25010000 0.20575800
O -2.30846200 1.86360300 0.68627200
H -2.90588500 1.44754300 0.05176500
H -1.43790100 1.83815800 0.26375200

$(H_2SO_4)(NH_3)(H_2O)_4$ [4-1] Cluster (2.43 kcal/mol), $\Delta\alpha$ = 26.39, $\bar{\alpha}$ = 87.86

S 0.89528300 -0.47431800 -0.26660000
O 1.97330100 -1.14567500 -0.91476500
O -0.26141800 -0.12829700 -1.06173300
O 0.45506200 -1.28252800 0.93619200
H -0.59056800 -1.15450700 1.21199900
O 1.41802300 0.86288900 0.31172300

H 2.45507100 0.81408400 0.42844300
N 3.98522800 0.54813900 0.44157100
H 4.56781000 1.26287600 0.02330400
H 4.01172700 -0.27595700 -0.15337900
H 4.38327300 0.30293000 1.33989600
O -1.89943900 -1.07409100 1.52261000
H -2.37682400 -1.58426600 0.85296500
H -2.24499000 -0.15177100 1.37077800
O -2.88510600 -1.07708600 -1.08578900
H -3.18492400 -1.51444400 -1.88408600
H -1.96282000 -0.81594500 -1.24447000
O -0.92426300 2.60946300 -0.48528600
H -0.63361500 1.79276700 -0.91532900
H -0.19642900 2.81759800 0.10579500
O -2.97338600 1.19413400 0.73874500
H -3.35188800 0.76455800 -0.03778600
H -2.31915300 1.82371900 0.38289500

$(H_2SO_4)(NH_3)(H_2O)_5$ [0-5] Cluster (3.75 kcal/mol), $\Delta\alpha = 9.81$, $\bar{\alpha} = 97.06$

S 1.74890900 0.02804200 -0.59427600
O 1.65553000 1.34819900 -0.01663600
O 2.53166100 -0.09631400 -1.77981200
O 2.48843300 -0.88076800 0.51577200
H 3.35757600 -1.10934400 0.16842500
O 0.41934900 -0.60195100 -0.65533300
H -0.70144700 0.57061100 0.15589200
N -1.43147800 1.07830000 0.68792200
H -1.95747400 0.36601800 1.20484000
H -2.06466000 1.53464400 0.00970300
H -0.96443500 1.75238400 1.31384900
O 0.00812300 -2.60035900 1.21934700
H 0.29187900 -2.03783300 0.47729400
H 0.72754100 -2.54091300 1.85139700
O -2.28930000 -0.98271200 -1.48376100
H -2.46164300 -1.35500100 -0.60740600
H -1.32754100 -0.99486700 -1.57314000
O -2.41971400 -1.52132400 1.36626900
H -3.09687100 -2.04399500 1.79833300
H -1.56904700 -2.00746800 1.46295100
O -3.26225500 1.55277200 -1.34263400
H -3.31195100 2.08071600 -2.14037400
H -3.01796100 0.64528500 -1.61202000
O 0.39772200 2.76175800 1.93645300
H 1.05529000 2.35807200 1.34287400
H 0.84215700 2.95051100 2.76304400

$(H_2SO_4)(NH_3)(H_2O)_5$ [1-4] Cluster (1.76 kcal/mol), $\Delta\alpha = 20.57$, $\bar{\alpha} = 96.88$

S -0.89788800 -0.34143500 -0.43252400
O 0.15399200 -0.78254400 0.47752900
O -1.69112700 -1.40496000 -0.98882900
O -1.86236700 0.54758900 0.45678800
H -2.69184200 0.04602700 0.64708800
O -0.36966000 0.60526400 -1.41138900

H 1.34410200 0.95212900 -0.93296600
N 2.14816600 1.24906800 -0.35272600
H 2.50410700 2.13240900 -0.70328800
H 2.87898800 0.50790200 -0.34830000
H 1.74875500 1.39993600 0.60423300
O 0.68127200 1.70821800 1.92828600
H 0.12597500 2.32824200 1.43307100
H 0.19560000 0.87383400 1.90671000
O -0.08569900 3.16023300 -0.38730600
H -0.69346000 3.88002100 -0.56311200
H -0.45139400 2.37893800 -0.83618300
O -3.91923600 -1.16334600 0.59245600
H -4.76071900 -0.95280800 0.18402900
H -3.38925100 -1.60846400 -0.08886900
O 2.09611300 -2.68730800 0.48493600
H 1.29261800 -2.13407800 0.45869600
H 2.08144000 -3.13544500 1.33174200
O 3.92086300 -0.87330600 -0.24855700
H 4.41192800 -1.22265600 -0.99367800
H 3.33899300 -1.60522100 0.05899600

$(H_2SO_4)(NH_3)(H_2O)_5$ [2-3] Cluster (1.88 kcal/mol), $\Delta\alpha = 17.20$, $\bar{\alpha} = 96.85$

S 0.56826400 -0.32366100 -0.47288900
O -0.76307600 -0.28541800 -1.07480200
O 1.50930900 -1.19869900 -1.10784700
O 1.09179500 1.14542100 -0.63290300
H 2.10464500 1.12064100 -0.61133400
O 0.45430700 -0.56211000 0.97926600
H -2.45317600 -1.53609300 0.74823700
N -2.18480700 -0.85328000 1.47932700
H -1.14503700 -0.71662500 1.39380300
H -2.42317200 -1.20156100 2.40120100
H -2.65908200 0.06368800 1.30496000
O -1.59560900 2.37872800 -0.95212800
H -1.36062000 1.47907800 -1.23494000
H -0.74250500 2.76678300 -0.73818300
O 3.06145600 -0.24136700 2.00761800
H 3.01468800 0.36349400 2.74971600
H 2.13923800 -0.44887600 1.77781200
O 3.63075800 0.72491100 -0.51006500
H 3.58266400 -0.08556500 -1.03114900
H 3.65380500 0.41174000 0.41494600
O -2.52324000 -2.35641500 -0.84565700
H -2.26180300 -3.23943200 -1.11104900
H -1.84805400 -1.75128000 -1.20133600
O -3.20100200 1.64720100 1.03868000
H -4.09778700 1.88413500 0.79722700
H -2.61996700 2.02338700 0.33373300

$(H_2SO_4)(NH_3)(H_2O)_5$ [3-2] Cluster (0.00 kcal/mol), $\Delta\alpha = 20.79$, $\bar{\alpha} = 96.57$

S -0.04969700 -0.22994000 -0.49215100
O -1.35964000 -0.36284400 -1.11393200
O 0.99503500 -1.00214700 -1.11481500

O 0.28422200 1.28440900 -0.66579800
H 1.23915600 1.47376900 -0.33730400
O -0.12605000 -0.47619800 0.95927800
H -1.61169200 -0.02125500 1.50917500
N -2.62647700 0.26643600 1.56170400
H -2.91127300 0.49708200 2.50634200
H -3.16972000 -0.52623300 1.17732100
H -2.72746000 1.08184600 0.91745600
O 2.64154700 1.63369400 0.20768400
H 3.24448300 1.14571400 -0.37083500
H 2.64758000 1.08363100 1.01855900
O 3.68182800 -0.83181100 -0.67444900
H 4.23225000 -1.34180800 -1.27012500
H 2.75774400 -0.99228500 -0.94216700
O -2.56012500 2.11547900 -0.49355500
H -1.76084500 2.64962500 -0.44695600
H -2.28608000 1.37673900 -1.06081900
O 2.55905200 -0.45590900 1.98239700
H 3.09329600 -0.94072700 1.34078000
H 1.64240200 -0.67972900 1.76435500
O -3.48707700 -1.75321000 -0.10125200
H -2.71186400 -1.49396600 -0.63069400
H -3.52782400 -2.71012300 -0.11706600

$(H_2SO_4)(NH_3)(H_2O)_5$ [4-1] Cluster (4.45 kcal/mol), $\Delta\alpha = 20.27$, $\bar{\alpha} = 96.24$

S 0.48665500 -0.68060000 -0.46711000
O 1.65684300 -1.47033200 -0.74634500
O -0.76553600 -1.18532100 -0.99297700
O 0.37284900 -0.68828200 1.10011300
H -0.44664900 -0.13282500 1.40830200
O 0.69354400 0.73732700 -0.84533300
H 2.24507900 0.87268700 -0.99284000
N 3.30481900 0.70605400 -0.91383900
H 3.87183100 1.44496600 -1.31053700
H 3.46376900 -0.19170000 -1.36898700
H 3.47923700 0.58583900 0.10646500
O -1.66525200 0.61858000 1.77847400
H -1.51272300 1.44925000 1.27292700
H -2.38914400 0.16629000 1.31755500
O -3.07451000 -1.56617600 0.53929500
H -3.02327300 -2.20582500 1.25539300
H -2.22812400 -1.66702500 0.06656500
O 3.01068400 0.16327800 1.72587200
H 3.22741400 0.29813600 2.64851900
H 2.08882800 -0.13898100 1.68458200
O -2.82545500 0.74274900 -1.19636400
H -3.59171000 0.19776200 -1.01029600
H -2.10724500 0.11216300 -1.35372000
O -1.34937200 2.71665200 0.01055400
H -0.48335800 2.40505900 -0.27467000
H -1.94448900 2.20364300 -0.56492500

$(H_2SO_4)(NH_3)(H_2O)_5$ [5-0] Cluster (5.22 kcal/mol), $\Delta\alpha = 22.75$, $\bar{\alpha} = 97.78$

S 1.29484900 -0.58631100 -0.26723200
O 2.58067100 -0.94010200 -0.77006800
O 0.13439100 -1.06572000 -0.98125700
O 1.19739900 -0.98714300 1.18707500
H 0.17280000 -0.85814900 1.61020800
O 1.16979100 0.96462600 -0.27071800
H 2.12459800 1.38586200 -0.17629000
N 3.62034900 1.77058700 -0.11437000
H 3.97294900 2.01344800 0.80344400
H 3.92422000 2.48193600 -0.76773900
H 4.03423700 0.88382400 -0.39043800
O -1.04377800 -0.67188700 2.05164300
H -1.62264900 -1.25463300 1.53213800
H -1.25756300 0.27347300 1.80771600
O -2.02910100 -2.38132800 0.07291800
H -2.15052600 -3.33178800 0.10384400
H -1.17286300 -2.21344200 -0.35658400
O -1.22166500 1.79580500 1.24406500
H -0.47641400 1.78163700 0.63215900
H -1.99984600 2.06454100 0.71708900
O -2.49594800 -0.07825300 -1.61871600
H -2.79135600 -0.87167300 -1.15709900
H -1.53287200 -0.15684600 -1.59822700
O -3.36600900 2.17626400 -0.38530500
H -3.55366100 2.89391700 -0.99093400
H -3.13709200 1.39667900 -0.93007000

$(H_2SO_4)(NH_3)(H_2O)_6$ [0-6] Cluster (10.94 kcal/mol), $\Delta\alpha = 20.88$, $\bar{\alpha} = 105.67$

S -2.45911400 -0.78886000 -0.19152300
O -1.29893300 -1.62601600 0.03578000
O -3.72139900 -1.45210600 -0.18202100
O -2.49802000 0.24258300 1.06601700
H -3.03289300 -0.15640500 1.76140600
O -2.23079000 0.13945500 -1.30003400
H -0.48324300 0.17532200 -1.56011900
N 0.50861100 0.31643500 -1.28108200
H 1.18184900 0.03025800 -1.98559400
H 0.67632100 -0.25156500 -0.43435100
H 0.65491100 1.30429800 -1.03971000
O 1.19574500 -1.19013800 1.16412700
H 0.87554900 -0.39106300 1.63057700
H 0.38980400 -1.69616900 0.98418800
O 0.20116200 1.23913100 1.86925900
H -0.69277600 1.27146200 1.50568200
H 0.72535400 1.84253500 1.32554400
O 2.18042600 2.20481000 0.00724800
H 2.72751100 2.99029200 -0.02221400
H 2.76874900 1.43054700 -0.09171900
O 3.20530800 -0.27277600 -0.45044800
H 2.67460400 -0.78543700 0.18490200
H 4.10856900 -0.61698700 -0.40382300
O -1.07092200 2.52294300 -0.54818600
H -1.50566500 3.35111200 -0.34229400

H -1.77179800 1.89059100 -0.77672900
O 5.83040800 -1.34748900 -0.24106400
H 6.00246800 -2.15994800 -0.72192200
H 6.14234600 -1.50530800 0.65269800

$(H_2SO_4)(NH_3)(H_2O)_6$ [1-5] Cluster (3.99 kcal/mol), $\Delta\alpha = 19.71$, $\bar{\alpha} = 106.31$

S 1.66200800 0.04267600 0.01784500
O 0.51964600 0.82043100 0.49543600
O 2.84203600 0.81664000 -0.24335500
O 1.96542700 -0.91480700 1.23807400
H 2.75778500 -1.43643200 0.98992800
O 1.27909100 -0.83058100 -1.09328300
H -0.38393700 -0.79623400 -1.22012200
N -1.41660600 -0.69912900 -1.05869100
H -1.99550300 -1.16638100 -1.75480400
H -1.67098900 0.29968200 -1.00697300
H -1.65075000 -1.12816400 -0.15444200
O -2.75801800 -1.69045200 1.33100300
H -2.53024600 -0.79872700 1.69215100
H -2.50322100 -2.33661500 1.99113300
O -3.90829500 -1.91435100 -1.20688500
H -4.75866600 -2.31072400 -1.39792500
H -3.78804900 -1.95741300 -0.24610400
O 4.08536000 -1.81580400 -0.27573200
H 3.50266100 -2.03869100 -1.00964900
H 4.26168900 -0.87519800 -0.41034700
O 0.03139500 3.34877700 -0.40007600
H 0.47442700 2.55222800 -0.05560300
H 0.26553900 4.06635400 0.19016400
O -2.26303200 2.03905800 -0.65404000
H -2.93959400 2.49279000 -1.15907400
H -1.48838200 2.64701200 -0.59451500
O -1.91546400 0.75606200 1.86343900
H -0.96857800 0.73815300 1.64860000
H -2.28523100 1.33967200 1.18625400

$(H_2SO_4)(NH_3)(H_2O)_6$ [2-4] Cluster (0.00 kcal/mol), $\Delta\alpha = 19.92$, $\bar{\alpha} = 105.87$

S 0.72531800 0.32046000 -0.16700100
O -0.66170900 0.67107700 -0.46623100
O 1.21351000 -0.78105400 -0.98349300
O 1.52502200 1.59399400 -0.53901100
H 2.51817600 1.43856600 -0.43246500
O 0.91189100 0.06890300 1.25966200
H -0.71645300 -0.64815800 1.81150000
N -1.56186100 -1.22553000 1.68194300
H -1.77522000 -1.75245100 2.52132400
H -1.34926700 -1.86819300 0.87741200
H -2.38094000 -0.61816300 1.39719800
O -3.66303800 0.19787000 0.76069300
H -3.42136000 1.14119800 0.74468500
H -3.62919500 -0.07369500 -0.16889700
O -2.43239300 2.61947800 0.34724900
H -2.14790500 3.41674300 0.79490700

H -1.62923000 2.14633800 0.07559300
O 3.39924800 -1.35291800 0.80272700
H 2.76714100 -1.01011100 1.44782100
H 2.81941600 -1.56113900 0.05664300
O -2.62217500 -0.64983700 -1.76653500
H -1.85982300 -0.10315900 -1.49141500
H -2.84811900 -0.38312000 -2.65936400
O 4.03547500 1.07061000 -0.21519800
H 3.99212700 0.16849800 0.17356200
H 4.54788700 0.99585600 -1.02262700
O -0.93890100 -2.61376700 -0.59569300
H -1.59081300 -2.24352500 -1.20842500
H -0.10392300 -2.18898300 -0.85240200

$(H_2SO_4)(NH_3)(H_2O)_6$ [3-3] Cluster (2.95 kcal/mol), $\Delta\alpha = 19.99$, $\bar{\alpha} = 105.48$

S 0.04398500 -0.65895500 -0.32006400
O -1.24753500 -1.15446600 -0.74700000
O 1.09831100 -1.64209300 -0.27719600
O 0.40611400 0.41173600 -1.39623400
H 1.34381700 0.78052200 -1.22327800
O -0.06190900 0.07685000 0.96070700
H -1.85501900 0.32536900 1.28909900
N -2.84773500 0.46569800 1.03584900
H -3.29665500 1.10255900 1.68442000
H -3.30214700 -0.46167800 1.01326400
H -2.82250200 0.88134000 0.06294100
O -2.41270200 1.56559800 -1.39462200
H -1.73929000 2.16741100 -1.03982700
H -1.90944500 0.87130400 -1.83735600
O -0.82849900 2.71792200 0.59634000
H -0.22811700 3.45971500 0.68823800
H -0.29996500 1.91583000 0.74038900
O 3.79027200 -1.24776400 -0.07012300
H 4.33164400 -2.02464200 -0.21552500
H 2.86354200 -1.52771700 -0.19041600
O -3.45262600 -2.18503200 0.48303300
H -2.62371400 -2.13074200 -0.02268100
H -3.46640100 -3.04454700 0.90509100
O 2.73796800 1.26582900 -0.81141300
H 2.73100400 1.25078300 0.16885100
H 3.36340000 0.55803900 -1.01881400
O 2.62513800 0.57816400 1.83999300
H 3.18455100 -0.17424200 1.60640500
H 1.71943700 0.24014600 1.79139500

$(H_2SO_4)(NH_3)(H_2O)_6$ [4-2] Cluster (0.26 kcal/mol), $\Delta\alpha = 24.65$, $\bar{\alpha} = 106.34$

S 0.20137200 -0.56594100 -0.11875400
O 1.40935200 -1.35935600 -0.07929900
O -1.02378900 -1.33466600 -0.20938800
O 0.18767800 0.19261900 1.23772600
H -0.72484700 0.73421500 1.38131600
O 0.26606700 0.46463700 -1.17415200
H 1.77166200 1.08786200 -1.18467000

N 2.76793100 1.38264600 -0.97319600
H 2.97166600 2.30626100 -1.33728500
H 3.41601200 0.68009500 -1.33929000
H 2.87740200 1.33439400 0.07545900
O -1.94847900 1.39088600 1.51134700
H -2.59527600 0.66678400 1.64156400
H -2.14105400 1.74268500 0.61424200
O -3.37926800 -0.94880700 1.45486200
H -3.84378800 -0.88420900 0.61084600
H -2.55990500 -1.39873600 1.20984400
O 2.96140700 0.76463000 1.64935700
H 2.04497500 0.49086200 1.81091300
H 3.44810700 -0.05369300 1.49380900
O -2.20705700 1.91727800 -1.14627200
H -2.82747600 1.22591900 -1.41751300
H -1.34043400 1.53338400 -1.34600000
O 4.03856100 -1.03198800 -0.45893700
H 3.11474000 -1.33986600 -0.37651800
H 4.56983000 -1.80353700 -0.66057500
O -3.38365400 -0.65562400 -1.42416700
H -3.64925500 -1.17423900 -2.18528300
H -2.49637600 -0.96850400 -1.16703700

$(H_2SO_4)(NH_3)(H_2O)_6$ [5-1] Cluster (5.40 kcal/mol), $\Delta\alpha = 18.21$, $\bar{\alpha} = 106.41$

S 0.42563900 -1.20712900 -0.30220900
O -0.34637900 -2.36175400 -0.68955900
O 1.73157500 -1.11286000 -0.89330200
O -0.43753300 0.01629600 -0.83657300
H -0.03390400 0.87246200 -0.49052300
O 0.45204100 -0.99807400 1.15828400
H -1.07139600 -0.54826300 1.60157800
N -2.09801500 -0.29773600 1.64164000
H -2.22746000 0.66490900 1.29027000
H -2.45217300 -0.38452000 2.58788700
H -2.58583200 -0.97400200 1.00629800
O 0.53267000 2.23981300 0.10046600
H -2.09461900 2.36314100 -0.38948000
H 1.30666700 1.93509700 0.65292300
O 4.15397800 0.11838500 -0.31504500
H 4.83636600 -0.53276100 -0.14621700
H 3.38546100 -0.38051500 -0.63863900
O -2.94887000 -2.25915200 -0.03715900
H -2.03576100 -2.42625500 -0.36029700
H -3.50205100 -2.20315900 -0.81778500
O 2.38120500 1.10245900 1.55451600
H 3.16709100 0.87815800 1.02398100
H 1.89752100 0.26584800 1.62424900
O -2.30628600 2.33554600 0.57197000
H -2.99526600 2.98695300 0.71564100
H -0.13116200 2.58646300 0.70610100
O -1.42933000 2.42807200 -1.98734200
H -1.31885100 1.51164800 -2.26517000
H -0.53332100 2.71315400 -1.76699400

$(H_2SO_4)(NH_3)(H_2O)_6$ [6-0] Cluster (3.32 kcal/mol), $\Delta\alpha = 20.62$, $\bar{\alpha} = 106.81$

S 1.26222500 -0.43044600 -0.38670400
O 2.20822000 -0.64496400 -1.44200400
O -0.10643800 -0.13808300 -0.84722000
O 1.25955800 -1.45709100 0.63900000
H -0.24499400 -1.77797400 1.38582800
O 1.67046600 0.92453500 0.32531000
H 2.68290700 0.89238400 0.47470900
N 4.25848900 0.48423000 0.45400200
H 4.99296900 1.17988300 0.47001100
H 4.26836300 0.01757700 -0.44926200
H 4.46807200 -0.21390900 1.15785600
O -1.18900300 -1.88208600 1.64721100
H -1.60014100 -2.29197800 0.87225600
H -1.77687700 -0.56635600 1.72621500
O -2.04369900 -1.97967000 -1.06569700
H -1.98725700 -2.61850800 -1.77844400
H -1.23662400 -1.42459800 -1.11082500
O -2.25071300 0.37073800 1.69649300
H -2.78736200 0.39468600 0.82731700
H -1.55233100 1.11445100 1.60816700
O -1.36974300 2.12831500 -1.42961200
H -1.15719000 2.60267600 -2.23505200
H -0.76692500 1.35551100 -1.37820700
O -3.42029600 0.40277800 -0.57033200
H -2.90891200 1.06639300 -1.06166000
H -3.15893600 -0.45779200 -0.93825000
O -0.58877100 2.25022900 1.28619300
H -0.87970500 2.56777000 0.41743800
H 0.28327500 1.85970200 1.10641300

$(H_2SO_4)(NH_3)(H_2O)_7$ [0-7] Cluster (3.99 kcal/mol), $\Delta\alpha = 8.06$, $\bar{\alpha} = 114.78$

S 1.85635700 0.16474600 -0.32732800
O 0.69797000 -0.46507000 -0.97248300
O 3.09636500 -0.49558100 -0.59549200
O 1.99233400 1.60017800 -0.93575400
H 1.16575800 2.12083200 -0.79534700
O 1.58099400 0.34216000 1.10913100
H 0.48276000 -0.93022800 1.50495600
N -0.06680300 -1.81696800 1.44891700
H -0.33655700 -2.12816900 2.37618000
H 0.55021800 -2.48685800 0.94771500
H -0.91594200 -1.62542100 0.89170700
O -1.58157200 0.76584200 -1.76392800
H -1.40858200 1.69132300 -1.54297400
H -0.70413100 0.34141500 -1.69912600
O -0.47863800 1.98323300 1.94338200
H 0.34558300 1.48265100 1.81701800
H -1.11094000 1.34310000 2.30216200
O -2.46470700 -0.87936500 0.23478600
H -3.11822500 -1.29464000 -0.34703100
H -2.12213700 -0.15969800 -0.33595200

O -3.77505500 -0.93937300 -2.19247000
H -3.89137900 -1.41549400 -3.01528400
H -3.08643100 -0.27640100 -2.35383700
O -2.09196400 -0.21561100 2.81636600
H -2.52229600 -0.41661300 1.96508800
H -2.78916100 -0.05698200 3.45514300
O 1.75224000 -3.06685700 -0.26675400
H 1.38179700 -2.55286800 -0.99675500
H 2.59698700 -2.61673000 -0.13165300
O -0.34399100 2.93441900 -0.48886300
H -0.53024900 2.65957400 0.44715800
H -0.29294900 3.89224700 -0.49771800

$(H_2SO_4)(NH_3)(H_2O)_7$ [1-6] Cluster (7.54 kcal/mol), $\Delta\alpha = 24.29$, $\bar{\alpha} = 114.93$

S 1.58847600 0.38062600 -0.33995500
O 0.44989300 1.02209300 0.30418900
O 2.81569300 1.13126100 -0.28851200
O 1.81833100 -0.92797900 0.54881800
H 2.76356700 -0.97203200 0.84210100
O 1.23372000 -0.12024300 -1.65903300
H -0.62766200 -0.16292700 -1.68124600
N -1.53441500 -0.31599700 -1.21349100
H -2.03703500 -1.09901200 -1.62533800
H -2.09389000 0.54552200 -1.17262200
H -1.29460100 -0.60417800 -0.25100500
O -0.92385900 -1.42739300 1.43595700
H -0.01220800 -1.11676600 1.50381200
H -1.49625200 -0.73698600 1.81264000
O -0.02745300 -2.68857400 -1.24597600
H 0.66719700 -2.08011400 -1.53227400
H 0.17223000 -2.82629700 -0.31620800
O 4.40455600 -0.63165900 1.07618900
H 4.71621700 -0.38801700 1.94972200
H 4.26448200 0.19976600 0.59434700
O -0.69589800 3.45801200 0.24367400
H -0.11967000 2.67240300 0.32408800
H -0.20886200 4.09075000 -0.28640600
O -2.86051600 2.11806300 -0.49999300
H -2.11235600 2.71917600 -0.26085700
H -3.58193700 2.67374000 -0.79864200
O -3.16145400 0.15310400 1.59222200
H -3.58374200 -0.56053300 1.09825500
H -3.17671900 0.92638900 1.01148600
O -3.17695100 -2.28621500 0.02514000
H -2.33663600 -2.41108500 0.49163200
H -3.58534000 -3.15157600 -0.03115400

$(H_2SO_4)(NH_3)(H_2O)_7$ [2-5] Cluster (3.57 kcal/mol), $\Delta\alpha = 25.99$, $\bar{\alpha} = 116.20$

S -1.55001300 -0.78405900 0.13130400
O -0.44762200 -1.62100500 0.59831200
O -2.76924900 -1.47293100 -0.16701300
O -1.81730800 0.17329000 1.34616400
H -2.77931400 0.47986200 1.29907100

O -1.10460200 0.08862000 -0.97315700
H 0.49744000 0.40220700 -1.20740300
N 1.49636600 0.47238700 -1.53387600
H 1.50284700 0.57143900 -2.54431100
H 1.95426100 -0.41138100 -1.29433000
H 1.99945300 1.27834400 -1.09786800
O 1.16369600 0.52139400 1.43895000
H 0.44452100 1.11872800 1.66459600
H 0.73566100 -0.34776400 1.42771700
O 2.84500300 2.59075900 -0.42106600
H 3.46742200 3.18823300 -0.83734500
H 3.33083900 2.13131900 0.30867500
O -3.29239700 1.82339900 -1.44341200
H -2.94653000 2.71715200 -1.42242900
H -2.51461800 1.23969300 -1.43184300
O 1.68070600 -2.35446500 -0.78212200
H 0.85219600 -2.18609200 -0.27538400
H 1.53293000 -3.15991500 -1.27997900
O -4.29725200 0.76214200 0.90540500
H -4.15199100 1.24168000 0.06803400
H -4.51177700 -0.13581000 0.62538500
O 4.09804800 -1.12673500 -0.37558700
H 3.36990200 -1.76910700 -0.34404200
H 4.90681500 -1.63424600 -0.46026900
O 3.88280100 1.04200300 1.46355400
H 2.99090300 0.83788500 1.78567400
H 4.11009900 0.26425500 0.93209800

$(H_2SO_4)(NH_3)(H_2O)_7$ [3-4] Cluster (0.00 kcal/mol), $\Delta\alpha = 23.04$, $\bar{\alpha} = 115.67$

S 0.53587900 -0.28748000 -0.68214800
O -0.67203500 -0.27845700 -1.48589300
O 1.63492600 -1.02860800 -1.24272700
O 0.96424300 1.22761600 -0.63703800
H 1.91580100 1.30427300 -0.23945100
O 0.25309300 -0.66589200 0.70887600
H -1.27996300 -0.12636100 1.18102700
N -2.22136700 0.29838600 1.35522100
H -2.11937700 1.03562800 2.04633300
H -2.89910600 -0.43166500 1.63001800
H -2.52187900 0.74084400 0.46547500
O -2.63283400 1.64456900 -1.12068300
H -2.28324000 2.47679700 -0.78119000
H -1.86186600 1.18651200 -1.49463900
O -0.89075100 2.76679700 0.85810300
H -0.49122500 3.56378900 1.21167100
H -0.17768000 2.30694900 0.38312100
O 4.23820000 -1.16752600 -0.43821700
H 4.82330800 -1.70560800 -0.97322700
H 3.35194300 -1.23444100 -0.83847200
O -3.29500400 -1.23739900 -1.13513000
H -2.34409300 -1.15343600 -1.30853600
H -3.67144000 -0.41628100 -1.46646500
O 3.24501400 1.32462700 0.43861100

H 3.11941900 0.70839100 1.19464000
H 3.88409200 0.84676100 -0.10829100
O 2.79156300 -0.81731000 2.04330800
H 1.89657700 -0.98267700 1.71144900
H 3.37240600 -1.32662900 1.46356800
O -4.09915700 -1.74926600 1.40808700
H -3.91442500 -1.78133100 0.44978400
H -4.12180900 -2.65373700 1.72264500

$(H_2SO_4)(NH_3)(H_2O)_7$ [4-3] Cluster (1.02 kcal/mol), $\Delta\alpha = 22.08$, $\bar{\alpha} = 115.98$

S 0.04819700 -0.38993500 -0.39825500
O 1.38267000 -0.87104100 -0.72773500
O -1.02193800 -1.19534900 -0.96160100
O -0.03051900 -0.52343900 1.15268800
H -1.00430600 -0.29022600 1.49417700
O -0.11914200 1.02378600 -0.72369000
H 1.33187600 1.83539200 -0.46031500
N 2.31081800 2.07047600 -0.16209000
H 2.47410700 3.07033300 -0.16235100
H 2.96898700 1.57028900 -0.79376400
H 2.42500300 1.65524900 0.79637800
O -2.33891300 -0.02446300 1.89368900
H -2.88512900 -0.71236500 1.46133500
H -2.65271600 0.82059000 1.51203900
O -3.52874000 -1.88079000 0.24600900
H -3.94395500 -1.32679900 -0.42513900
H -2.65603600 -2.05830600 -0.13180800
O 2.42306100 0.61647400 2.13681100
H 1.54092600 0.21961200 2.07297500
H 3.01927500 -0.10773300 1.89121200
O -3.27585800 2.09711500 0.45068600
H -4.19159600 2.34992200 0.57927800
H -3.25061200 1.60141600 -0.38768100
O 3.63785900 -1.43817200 0.64124600
H 2.75525300 -1.45239300 0.22207800
H 3.85025800 -2.34303300 0.87650700
O -3.21370900 0.29615600 -1.67921300
H -2.35709300 -0.15186400 -1.53264700
H -3.20666300 0.58133900 -2.59473200
O 3.79193100 0.27048500 -1.68566200
H 4.21775000 -0.27674500 -1.01240200
H 2.96417200 -0.20515400 -1.84423000

$(H_2SO_4)(NH_3)(H_2O)_7$ [5-2] Cluster (4.11 kcal/mol), $\Delta\alpha = 19.59$, $\bar{\alpha} = 115.83$

S -0.50400300 0.19802700 -0.30250200
O -1.68723200 0.99264900 -0.55272300
O 0.65330500 0.53714500 -1.09238800
O -0.16103700 0.54908200 1.19944500
H 0.64981000 0.02009200 1.51062500
O -0.79287400 -1.24144200 -0.32620500
H -2.43464000 -1.46064500 0.01223900
N -3.42706000 -1.25481700 0.28341800
H -3.92852900 -2.09506500 0.54768800

H -3.87154200 -0.77655300 -0.52249900
H -3.36278900 -0.58347100 1.08008400
O 1.89832500 -0.84034900 1.83197400
H 1.96005800 -1.27332000 2.68557800
H 1.90240600 -1.56321600 1.11657000
O 2.23558900 2.71507300 -0.18297000
H 1.74250900 3.12616900 0.52902500
H 1.62592000 2.07101200 -0.57424700
O -2.82454700 0.58999200 2.26943100
H -3.17230800 1.45707400 2.04508300
H -1.87822600 0.65267700 2.05981800
O 3.15227800 -0.87722000 -1.76769800
H 3.63335500 -0.35950300 -1.09420300
H 2.37024700 -0.34049900 -1.94050300
O 1.79996600 -2.49819600 -0.10497900
H 2.36006100 -2.04354500 -0.77900100
H 0.89049000 -2.33954200 -0.39142600
O 4.02958800 0.61329900 0.41986500
H 3.45661500 0.17480100 1.06028100
H 3.58956000 1.46234100 0.25658400
O -4.06749500 0.48188400 -1.75171900
H -3.18036200 0.84395100 -1.57951800
H -4.18608600 0.46718700 -2.70234100

$(H_2SO_4)(NH_3)(H_2O)_7$ [6-1] Cluster (7.31 kcal/mol), $\Delta\alpha = 21.89$, $\bar{\alpha} = 117.11$

S -1.06870600 0.40330600 -0.31254800
O -2.21187300 1.22528000 -0.65626700
O 0.21768400 0.95779500 -0.68634300
O -1.11403400 0.25457300 1.21966500
H -0.28661400 -0.33152700 1.58797400
O -1.22316800 -0.96169200 -0.87689500
H -2.72091400 -1.20792400 -0.96654100
N -3.80686000 -1.15201800 -0.94697800
H -4.24678000 -2.06321200 -1.01117500
H -4.09792600 -0.56222800 -1.72176800
H -4.05498900 -0.65852000 -0.05329200
O 0.74930600 -1.12791400 2.00585200
H 1.00528700 -1.69838700 1.24132500
H 1.54934200 -0.63432700 2.27833300
O 1.98039900 3.10340600 -1.03415100
H 1.90582100 3.58822000 -1.85703400
H 1.15926200 2.59471000 -0.95111300
O 1.15032900 -2.44343400 -0.27582100
H 0.43190400 -2.02072700 -0.76488500
H 1.96404800 -2.33113700 -0.79537500
O 2.93896000 0.59925000 -0.30597300
H 3.00176900 1.50976400 -0.63656600
H 1.98072700 0.43695400 -0.36125300
O 3.03750100 0.30098500 2.44645600
H 2.99402900 1.14993800 2.88944100
H 3.17230400 0.49793700 1.50166800
O 3.56403300 -1.80512400 -1.53025400
H 3.54513700 -0.89252900 -1.19507300

H 3.71059600 -1.74167900 -2.47471500
O -4.10986000 0.48288900 1.21743800
H -3.60336700 0.21921600 1.99161200
H -3.49653300 1.06856600 0.73838900

$(H_2SO_4)(NH_3)(H_2O)_7$ [7-0] Cluster (7.00 kcal/mol), $\Delta\alpha = 21.02$, $\bar{\alpha} = 117.61$

S 1.29602700 -0.77678200 -0.09386100
O 2.22455700 -1.46428400 -0.94168900
O 0.05625900 -0.35563700 -0.73242000
O 0.99578300 -1.50924800 1.14834400
H -0.33418000 -1.49399000 1.52752400
O 1.98378400 0.55929000 0.36124300
H 3.00099600 0.51505200 0.18672700
N 4.50055900 0.22405700 -0.23080600
H 4.95505300 0.89697000 -0.83493400
H 4.30907200 -0.61714500 -0.76955500
H 5.14110800 -0.01409600 0.51592400
O -1.36445600 -1.45635700 1.79987100
H -1.63673500 -0.48918200 1.84187600
H -1.92296100 -1.92739900 1.08811300
O -2.09003400 -1.35171000 -2.23241600
H -2.46697200 -0.46505200 -2.15401500
H -1.15930200 -1.20724400 -2.00269800
O 0.05103600 2.46691300 1.18672400
H 0.79402900 1.91570100 0.89858300
H -0.16853400 3.05307400 0.43998800
O -2.11589300 1.29955600 -1.03800200
H -1.26001300 0.85657800 -0.89142500
H -2.52648900 1.27467500 -0.16461600
O -1.99784700 1.05160200 1.82989600
H -2.37178000 1.39248600 2.64494900
H -1.18446900 1.61100700 1.62046800
O -0.86253600 3.76641600 -1.06744400
H -1.45229100 3.01253100 -1.24434900
H -1.38255400 4.56271700 -1.17878000
O -2.78502400 -2.55081000 0.00680100
H -2.57233200 -2.15812700 -0.88128300
H -2.76701800 -3.50428800 -0.09235500

$(H_2SO_4)(NH_3)(H_2O)_8$ [0-8] Cluster (0.79 kcal/mol), $\Delta\alpha = 12.70$, $\bar{\alpha} = 124.42$

S -2.40311900 -0.24141800 -0.28685600
O -0.94378200 -0.49644900 -0.34612200
O -3.19610700 -1.35998800 -0.66438800
O -2.68507300 -0.02552600 1.25675600
H -2.17333600 0.75289000 1.55404800
O -2.70894800 1.01985300 -0.94662200
H 0.80666800 1.38854700 -1.16706800
N 1.53213100 0.67465000 -1.01451700
H 2.48056700 1.03033300 -1.22672700
H 1.31543000 -0.14949500 -1.58327200
H 1.48663100 0.40054100 -0.01665500
O -0.04445000 -2.03491800 1.70717900
H -0.71572000 -2.47217900 2.23409900

H -0.51329000 -1.57729200 0.97978300
O -0.93585900 2.12428900 1.70352400
H -0.81519400 2.44522600 0.78690500
H -1.19398100 2.88313700 2.23120900
O 3.96654800 -0.21038000 0.97637200
H 3.51782600 -0.99931600 0.62750900
H 3.30872700 0.17171300 1.57145000
O 2.22398800 -2.19396200 0.05217200
H 1.78535400 -2.34009100 -0.79604000
H 1.55643100 -2.41711200 0.71549900
O -0.64279000 2.56750400 -0.98818100
H -0.79329100 3.38411400 -1.46767400
H -1.46279000 2.00506100 -1.09727300
O 0.50578200 -1.81913700 -2.17090100
H -0.25501100 -1.52658200 -1.63213400
H 0.15407500 -2.25793400 -2.94677200
O 1.31790500 0.39166300 1.85320900
H 0.61754900 1.04483100 1.99652600
H 0.90197200 -0.46609200 2.03861400
O 4.19732200 1.48436500 -1.07816500
H 4.31539300 0.88333300 -0.30856800
H 4.96468300 1.37801400 -1.64080200

$(H_2SO_4)(NH_3)(H_2O)_8$ [1-7] Cluster (2.03 kcal/mol), $\Delta\alpha = 14.56$, $\bar{\alpha} = 123.86$

S 1.94377400 -0.09342900 0.14727200
O 1.99202200 -1.47755700 -0.27018800
O 3.17094700 0.46818100 0.63814300
O 1.61194200 0.68473600 -1.21810300
H 1.77163900 1.63858300 -1.06363300
O 0.79539100 0.17245200 1.01531000
H -1.63539400 -0.46636300 0.14311600
N -2.10881400 -0.14342900 1.00331100
H -1.92245200 0.85733100 1.09412200
H -1.69816800 -0.64702100 1.81526700
H -3.12460700 -0.26483100 0.90630500
O -1.00395300 -0.40327100 -1.66344700
H -0.18936400 0.11853300 -1.62855100
H -0.70755700 -1.27604500 -1.96923000
O -0.69865000 2.34216300 0.33124600
H -0.19132900 3.15463600 0.40654800
H -0.06706500 1.64099200 0.58187100
O 2.25991800 3.04349800 0.05206200
H 2.84127300 3.74996300 -0.23582600
H 2.81710000 2.41391000 0.53974500
O -0.52052600 -2.67647100 0.55285400
H 0.32782400 -2.23831500 0.38501400
H -0.59044200 -3.30791500 -0.16882800
O -0.61988900 -1.38906400 3.01745800
H -0.55976200 -2.21839400 2.52431700
H 0.15250600 -0.89248000 2.71628300
O -4.69934200 0.48612800 0.22912600
H -4.22616800 0.99820400 -0.45630600
H -5.56613400 0.27614500 -0.11810400

O -2.88491800 1.66468300 -1.42446600
H -2.20106500 2.13054900 -0.92277200
H -2.40521100 0.91979300 -1.81405200
O 0.45124800 -2.75159300 -2.18592700
H 1.18550500 -2.35900300 -1.68369100
H 0.81666200 -3.04049300 -3.02366500

$(H_2SO_4)(NH_3)(H_2O)_8$ [2-6] Cluster (2.29 kcal/mol), $\Delta\alpha = 23.39$, $\bar{\alpha} = 124.17$

S -1.91451400 -0.77383800 -0.49812600
O -1.04368400 -1.90003400 -0.81995600
O -3.28271100 -1.10880500 -0.19924700
O -1.26979000 -0.25676800 0.87052200
H -1.90912500 0.33147100 1.31483700
O -1.75691800 0.30185100 -1.46020800
H 1.94035500 -0.71610100 -1.34690900
N 1.11395800 -0.19545900 -1.73649100
H 1.32372900 0.17223200 -2.65845900
H 0.86173900 0.59785900 -1.10570700
H 0.30752400 -0.83084900 -1.77772700
O 1.53361800 0.10638800 1.91854300
H 1.18556500 -0.77368400 1.71140900
H 2.49091500 0.06014600 1.79579700
O 0.74830100 1.90431300 0.08003100
H -0.15028700 2.29536400 0.10120100
H 0.85801200 1.32429900 0.86380300
O -1.81708400 2.75994400 -0.18566300
H -2.49421800 2.62855600 0.48683800
H -1.95512000 2.01635500 -0.79653300
O 0.87904100 -2.53941900 0.96865000
H 0.10336900 -2.39713800 0.38531700
H 0.65401400 -3.27046100 1.54640400
O -3.63924200 1.09930800 1.43873300
H -4.18644800 1.06086900 2.22491500
H -3.91876500 0.36203700 0.86748900
O 3.04745500 -1.72974500 -0.58956600
H 3.64162300 -1.20247100 -0.03474200
H 2.46224800 -2.21105200 0.01742800
O 3.20244100 2.03081400 -0.88279400
H 2.30962400 2.22333300 -0.52116700
H 3.57925700 2.86899600 -1.15465900
O 4.23097100 0.29247800 0.93171400
H 4.00252900 1.00819000 0.30292900
H 5.06880300 0.51907600 1.33692200

$(H_2SO_4)(NH_3)(H_2O)_8$ [3-5] Cluster (0.00 kcal/mol), $\Delta\alpha = 26.59$, $\bar{\alpha} = 125.33$

S -0.90374600 0.40153900 -0.08109500
O 0.46329100 0.78779300 -0.38465300
O -1.84628400 1.49386000 -0.04928500
O -1.28862200 -0.51839600 -1.29892600
H -2.26829600 -0.82640200 -1.21374000
O -0.96266800 -0.44294900 1.11104300
H 0.79950100 -1.03842000 1.49690800
N 1.77435000 -1.07863300 1.16937000

H 2.40106000 -1.67641700 1.70427000
H 2.17760500 -0.12687100 1.17839500
H 1.74827000 -1.39752600 0.19191000
O 3.49430900 -0.43912000 -1.31170500
H 2.73668400 -0.89644700 -1.69845500
H 3.32453600 0.50198800 -1.44791500
O 1.10771000 -1.96259800 -1.54613500
H 0.97110400 -2.84952800 -1.88386600
H 0.25211600 -1.50437800 -1.61661100
O -4.55229400 1.22944100 0.16531300
H -5.03729400 2.05473200 0.12682000
H -3.60588600 1.45950600 0.09908400
O 2.52735700 2.24944100 -1.12277600
H 1.61967200 1.90514100 -1.00395600
H 2.47149700 3.06386700 -1.62379400
O -3.70002100 -1.20944300 -0.96936200
H -3.74622100 -1.40109600 -0.00762500
H -4.23575000 -0.40666000 -1.04015900
O -3.68223000 -1.03758800 1.75274600
H -2.74201100 -0.80387300 1.77706500
H -4.14295800 -0.19556000 1.64711200
O 3.18091100 1.42064600 1.42956900
H 3.07219600 1.86100000 0.56748600
H 2.85539500 2.04650900 2.08002300
O 4.55576700 -1.22726200 1.21380200
H 4.38202300 -1.05121000 0.27552100
H 4.62842200 -0.34314200 1.58641300

$(H_2SO_4)(NH_3)(H_2O)_8$ [4-4] Cluster (1.83 kcal/mol), $\Delta\alpha = 28.10$, $\bar{\alpha} = 125.53$

S -0.33993400 -0.41198200 0.16718500
O 0.73360500 -1.19173200 0.76931300
O -1.59559200 -1.12936600 0.07388200
O -0.52563600 0.78953000 1.12982900
H -1.17589800 1.48263700 0.71542400
O 0.06349900 0.14813900 -1.13114200
H 1.53949000 -0.61746600 -1.55056200
N 2.45866900 -1.11519900 -1.56394200
H 2.45110800 -1.86100100 -2.25111300
H 2.59527900 -1.49836000 -0.62415100
H 3.25240300 -0.43925600 -1.72830200
O -2.08697700 2.42859900 0.05249000
H -2.97781900 2.00274800 -0.10232900
H -1.74885100 2.67368600 -0.81193400
O -4.10710400 -1.14539500 1.21943800
H -4.19810400 -1.49092400 2.10839200
H -3.15825900 -1.17373200 1.00959500
O 2.29766000 1.82236400 -0.26273900
H 1.43853400 1.54967400 -0.61021100
H 2.29290100 1.53150300 0.66081800
O -4.36036200 1.19469800 -0.32127200
H -4.48621200 0.61222700 0.44225000
H -4.22759000 0.55209700 -1.04053000
O 2.43212600 0.32508100 2.19171000

H 1.69651600 -0.22999600 1.85676000
H 2.17462500 0.64759800 3.05665700
O -3.76213500 -1.12262200 -1.77572200
H -4.28670000 -1.63377100 -1.15100800
H -2.87201000 -1.15677700 -1.39638700
O 4.27907700 -1.06110700 0.72840300
H 3.77051000 -0.56244700 1.39367700
H 4.80028500 -1.69782400 1.22039700
O 4.46125800 0.70227600 -1.54809800
H 3.83689900 1.33862100 -1.15173000
H 4.87580300 0.28515500 -0.78180500

$(H_2SO_4)(NH_3)(H_2O)_8$ [5-3] Cluster (3.98 kcal/mol), $\Delta\alpha = 27.88$, $\bar{\alpha} = 125.75$

S -0.38373200 -0.33222000 -0.03300600
O -1.54379300 -0.47773700 -0.89088100
O 0.76023600 -1.14854200 -0.42444500
O 0.03360200 1.15413100 -0.19688900
H 0.92591000 1.35683800 0.36396600
O -0.70840700 -0.53956300 1.38031300
H -2.32140700 -0.28289800 1.57701500
N -3.35339500 -0.08970400 1.46276100
H -3.82295100 -0.00094700 2.35691800
H -3.76597500 -0.84652200 0.90069300
H -3.44875400 0.77886600 0.91756900
O 2.09288700 1.53682800 1.09021100
H 2.28128700 0.69383900 1.53712300
H 2.85943900 1.68693300 0.47598100
O 4.10574500 1.67223600 -0.62807400
H 4.62931800 0.93699900 -0.26634100
H 3.67911800 1.25368800 -1.38857100
O -2.53308800 2.30996900 0.03877400
H -2.55705500 3.25833800 0.17527900
H -1.60442400 2.07728500 -0.12445500
O 2.86654300 -0.47732400 -2.06384800
H 2.73801700 -0.78259700 -2.96322100
H 2.04273000 -0.68605500 -1.58675600
O 2.43908200 -1.17935600 1.78606000
H 2.04854500 -1.54413900 2.58247100
H 1.80490500 -1.36538300 1.06979800
O 4.77186100 -0.95820000 0.07917800
H 4.18097500 -1.18309000 0.80878100
H 4.24087000 -1.10382700 -0.71519400
O -3.73166200 -1.98485100 -0.62842400
H -2.83733800 -1.66481300 -0.85654900
H -3.78008600 -2.90903900 -0.87538600
O -4.70626100 0.73831800 -0.94925100
H -3.91492400 1.24985600 -1.15349600
H -4.53868900 -0.14717200 -1.28864100

$(H_2SO_4)(NH_3)(H_2O)_8$ [6-2] Cluster (4.11 kcal/mol), $\Delta\alpha = 23.85$, $\bar{\alpha} = 125.95$

S 0.74040700 -0.26236600 -0.56041100
O 1.97505100 -0.27923400 -1.31007000
O -0.43851800 -0.64167100 -1.29668800

O 0.97482800 -1.35396600 0.54646700
H 0.11578900 -1.57125300 1.04482100
O 0.55975500 1.00979100 0.15655400
H 1.99095300 1.59662400 0.63742300
N 2.99752800 1.73891800 0.93987700
H 3.33342200 0.79907800 1.26661500
H 3.07665400 2.44989400 1.65794000
H 3.57396200 1.95790700 0.12230900
O -1.22602900 -1.92170800 1.71181500
H -1.21007300 -2.33563000 2.57663300
H -1.85556400 -1.12483100 1.76263800
O -2.28672000 -2.87039300 -0.86330200
H -2.05125500 -2.79250100 0.07007200
H -1.51977700 -2.48908500 -1.30701600
O -1.74598600 2.42885200 1.05003100
H -0.97641800 2.05803200 0.59802400
H -2.39883100 2.62207100 0.35722200
O -3.21582300 -0.23027100 -1.11707600
H -3.31921300 -1.19371000 -1.16698200
H -2.26018500 -0.12622800 -1.25293200
O -2.85876400 0.02891600 1.66309300
H -2.44846700 0.92013200 1.64870100
H -3.19302200 -0.06624900 0.75464200
O -3.80294100 2.47896600 -0.89266900
H -3.84016200 1.53238400 -1.10051800
H -4.68469300 2.72267300 -0.60737100
O 4.45653200 0.71868500 -1.19386100
H 4.96785200 0.79169500 -2.00101700
H 3.58597700 0.35324900 -1.44364000
O 3.75054200 -0.85809100 1.21660200
H 4.23777500 -0.85918100 0.38356600
H 2.91065200 -1.29865900 1.01916500

$(H_2SO_4)(NH_3)(H_2O)_8$ [7-1] Cluster (12.20 kcal/mol), $\Delta\alpha = 18.76$, $\bar{\alpha} = 125.26$

S -1.50178000 -0.63052200 -0.55318500
O -2.90314300 -0.93955100 -0.66825600
O -0.58635700 -1.54090300 -1.18734300
O -1.36172800 0.77766600 -1.25967700
H -0.45125000 1.16016400 -1.04343500
O -1.11843800 -0.36876500 0.85798600
H -2.49063700 -0.00718700 1.57230800
N -3.52731900 0.21367900 1.72449200
H -3.73773000 0.51797500 2.66818900
H -4.03392000 -0.63457300 1.48150100
H -3.76116300 0.94299500 1.00738300
O 0.94197800 1.65191400 -0.53189500
H 1.22480900 1.07738900 0.20016300
H 1.68155000 1.55198600 -1.16631900
O 3.23650000 0.88231300 -1.70102800
H 3.77809100 0.99144600 -2.48297000
H 2.91017300 -0.06704000 -1.68418600
O 0.29520000 -2.82265600 1.40850200
H 0.13527700 -3.13711800 0.51312300

H -0.12558100 -1.95171100 1.40405300
O 2.27278000 -1.48226200 -1.38774700
H 1.30507800 -1.51411000 -1.37826100
H 2.56910300 -1.79110500 -0.50372300
O 3.03250800 0.74188100 1.15378500
H 2.99642900 1.63749000 1.51713400
H 3.46614500 0.83427900 0.29347100
O 3.00216300 -2.10125600 1.16552900
H 3.06071100 -1.19164100 1.48611900
H 2.13117600 -2.42410600 1.44887900
O 2.11991600 3.41797200 1.41841800
H 1.60286300 3.15438400 0.64487600
H 2.48888800 4.27870100 1.21592400
O -3.76281200 1.99372600 -0.34956400
H -2.93402800 1.71418700 -0.77672300
H -4.44481600 1.76955900 -0.98766900

$(H_2SO_4)(NH_3)(H_2O)_8$ [8-0] Cluster (6.19 kcal/mol), $\Delta\alpha = 29.50$, $\bar{\alpha} = 126.59$

S -2.01642200 -0.72958000 -0.01144700
O -3.20706600 -1.50858200 -0.07440900
O -1.02727900 -1.04722600 0.98293300
O -1.36757700 -0.73380700 -1.39175300
H -0.40871500 -0.28266100 -1.35431100
O -2.38970300 0.75174900 0.24642800
H -3.33345500 0.95195100 -0.16375800
N -4.75291600 0.99133400 -0.76574900
H -5.45032600 1.48488600 -0.22224900
H -4.98649000 0.00205800 -0.76493000
H -4.80145500 1.32670200 -1.72030800
O 0.81661600 0.37920100 -1.15348300
H 1.64904300 0.11560000 -1.63329600
H 1.07434400 0.30938900 -0.20925400
O 1.23369900 -2.41672600 1.53501600
H 1.11002000 -3.04705100 2.24668300
H 0.34662800 -2.09490700 1.28792800
O -0.18385700 2.04098700 1.85639300
H -0.99802800 1.65912600 1.50922500
H 0.16001600 2.61199800 1.14542400
O 1.81019600 0.34726700 1.42051900
H 1.74029900 -0.55616800 1.75596400
H 1.05581800 0.87617500 1.77620000
O 3.22652700 -0.23159900 -1.95936500
H 3.34695500 -1.06643900 -1.47356200
H 3.65487100 0.44991000 -1.42160100
O 1.12613500 3.15449700 -0.35815900
H 2.07068500 3.00040000 -0.22145000
H 0.86974400 2.42510400 -0.93673400
O 3.20421800 -2.59343500 -0.47198800
H 3.07520100 -3.39627700 -0.97949000
H 2.50710700 -2.59247600 0.20358100
O 3.66423700 1.76694500 0.05702800
H 4.45818500 2.04744000 0.51526200
H 3.14355900 1.23499200 0.69079300

$(H_2SO_4)(NH_3)(H_2O)_9$ [0-9] Cluster (4.87 kcal/mol), $\Delta\alpha$ = 19.23, $\bar{\alpha}$ = 134.27

S -2.87858400 -0.05300000 -0.62363600
O -2.03661300 -1.13461800 -0.12307100
O -3.88409100 -0.41887000 -1.56596100
O -3.63447100 0.41275300 0.71186400
H -4.49876200 0.76274200 0.46832300
O -2.06497900 1.10201000 -1.00667000
H -0.38398200 0.68614200 -0.89353800
N 0.55354500 0.39583100 -0.54668300
H 1.31784600 0.58595200 -1.22214100
H 0.52566700 -0.60652600 -0.32586300
H 0.72932500 0.92538800 0.30515200
O -0.78148200 -0.35625900 2.27786000
H -0.79531000 0.61171000 2.17971700
H -1.39193600 -0.68378900 1.59775800
O -0.88944500 2.27814300 1.39583600
H -0.15115300 2.81036700 1.07148500
H -1.47630400 2.14052300 0.63787000
O 3.06826800 -0.79810200 0.78380600
H 2.52935500 -1.23994400 1.46257900
H 3.10814200 -1.39580000 0.02378800
O 2.63662300 -2.18930000 -1.64401600
H 1.75327700 -2.44266900 -1.31257400
H 3.00163400 -2.96234400 -2.07791300
O 1.53596800 3.11526900 0.10448700
H 2.43130200 2.74895400 0.20182100
H 1.53996000 3.61170900 -0.71600100
O 2.80168200 0.64097300 -2.19727700
H 2.96169700 -0.31217400 -2.22888000
H 3.45841400 1.00763900 -1.59005600
O 1.19070900 -2.03062600 2.37994500
H 1.25211900 -2.48820600 3.21964100
H 0.46706100 -1.35118900 2.46119200
O 3.90165800 1.65295000 0.23292000
H 4.72780100 1.90055500 0.65098400
H 3.65530600 0.76477500 0.57786400
O 0.34298200 -2.52611600 -0.23492400
H 0.53360500 -2.64136600 0.70963500
H -0.60700200 -2.34092500 -0.31428000

$(H_2SO_4)(NH_3)(H_2O)_9$ [1-8] Cluster (5.71 kcal/mol), $\Delta\alpha$ = 13.86, $\bar{\alpha}$ = 134.46

S 2.13982000 -0.40721500 -0.56217200
O 1.73167700 0.99072900 -0.57782600
O 3.49703000 -0.63971500 -0.14732400
O 1.20759200 -0.99623600 0.61540000
H 1.62078400 -1.83055200 0.94823100
O 1.73422200 -1.11732000 -1.75628600
H -0.05674800 -1.03644900 -1.79048200
N -1.02160800 -0.83487300 -1.47231800
H -1.74211700 -1.14412400 -2.12476400
H -1.12473700 0.18550500 -1.29986800
H -1.21329800 -1.32747000 -0.57723600

O -2.15382900 -2.16181600 0.70902300
H -2.92109600 -2.28920000 0.13465400
H -2.44828300 -1.56371500 1.41130500
O -3.75486400 -1.62661200 -1.59141000
H -4.56583700 -1.88001100 -2.03406900
H -3.93598400 -0.77624100 -1.12720600
O 2.88634000 -2.96652500 1.24726700
H 3.51552700 -2.38448000 0.79200400
H 2.89225200 -3.79570000 0.76510600
O 1.60478600 2.86271200 1.34267100
H 1.88001700 2.16628000 0.71257300
H 2.39095800 3.12554600 1.82477800
O 0.59940400 3.46349100 -1.37599300
H 0.87857300 3.77651700 -0.50718500
H 1.15852300 2.68764500 -1.51681000
O -1.44729900 1.80971400 -0.63626500
H -1.08655400 1.61793000 0.24699800
H -0.85340400 2.49940500 -0.99738000
O -3.92472200 0.63526800 -0.18389300
H -3.73959200 0.48000100 0.75377900
H -3.24103800 1.26443600 -0.46151700
O -0.36918800 0.97507300 1.83558200
H 0.19177500 0.24715400 1.51785200
H 0.24102500 1.71992400 1.96827200
O -2.83679600 0.03040200 2.39317800
H -3.16403800 0.08734200 3.29214600
H -1.95739800 0.45649600 2.37679900

$(H_2SO_4)(NH_3)(H_2O)_9$ [2-7] Cluster (5.40 kcal/mol), $\Delta\alpha = 22.21$, $\bar{\alpha} = 133.54$

S -1.80013200 -0.95270400 -0.20901200
O -0.89293400 -2.07202600 -0.06751300
O -3.20518500 -1.26997300 -0.19987100
O -1.52692500 -0.07951400 1.09432900
H -2.35067600 0.37176200 1.36706800
O -1.41072400 -0.10748900 -1.34239100
H 0.16286200 -0.93282100 -1.93041800
N 1.14525100 -1.01779600 -2.22944600
H 1.20494800 -1.51201500 -3.11250000
H 1.73394600 -1.50234400 -1.47424700
H 1.52237100 -0.05818600 -2.30063700
O 2.14867900 1.47544000 -1.48573500
H 1.52580300 2.21116800 -1.54833600
H 2.01511400 1.16933500 -0.56722900
O -0.33359600 2.37133400 -0.50650800
H -1.17313400 2.83765900 -0.39836600
H -0.63668100 1.51829900 -0.85754000
O -3.15868300 2.30445400 -0.73819900
H -3.72619900 1.99085200 -0.02488700
H -2.95530900 1.51493700 -1.25290300
O 1.02512500 -1.84270700 1.79946100
H 0.23935900 -2.05894400 1.25845500
H 0.88555000 -2.21108800 2.67294100
O -4.18479900 0.66140000 1.40884700

H -4.78820300 0.58059800 2.14900900
H -4.24464300 -0.15699400 0.88577800
O 2.78072900 -1.95712800 -0.38694300
H 3.46146900 -1.25308700 -0.32003600
H 2.36766300 -2.03718100 0.48562300
O 4.49139300 0.17193100 -0.41477300
H 4.09765700 0.80715300 -1.02314900
H 4.48374500 0.62642200 0.44551000
O 3.91690400 1.43431800 1.99583900
H 2.96083300 1.38916200 1.82618200
H 4.10811600 2.33292000 2.26657700
O 1.37570000 0.83980100 1.09880700
H 0.56172900 1.33784800 0.92416500
H 1.12355700 -0.03633500 1.43645500

$(H_2SO_4)(NH_3)(H_2O)_9$ [3-6] Cluster (1.46 kcal/mol), $\Delta\alpha = 24.35$, $\bar{\alpha} = 134.88$

S 0.66972500 -0.67550500 -0.06424200
O -0.76302900 -0.94771700 -0.01475200
O 1.49684400 -1.84800400 -0.12583200
O 0.83469400 0.13222600 -1.38888600
H 1.71557300 0.68373200 -1.39682600
O 1.06019700 0.23415100 1.02719800
H -0.45259200 1.38772900 1.08066500
N -1.18665700 2.04683000 0.79127400
H -0.89836700 2.98250000 1.05989000
H -2.10528800 1.74995700 1.19191500
H -1.28931500 1.97010500 -0.25730300
O -1.61156100 1.59196000 -1.84160200
H -2.44528400 1.09301300 -1.81468900
H -0.90890600 0.94855700 -2.00369200
O 1.63188600 2.94718300 0.90143100
H 2.29307200 3.29899100 1.50159900
H 1.63205200 1.98541500 1.03882800
O 3.96840400 0.21196000 0.79589000
H 4.31561400 -0.65052800 0.50589600
H 3.11450700 -0.00430100 1.19237400
O -2.52563100 -1.64535300 1.94074900
H -1.72911500 -1.44789300 1.41370900
H -2.23258500 -2.10012800 2.73209800
O 4.24468600 -2.38316800 -0.12872500
H 4.57522500 -2.63173100 -0.99310500
H 3.27799300 -2.35800400 -0.21086800
O 2.91963200 1.52546400 -1.28263600
H 3.44735500 1.07799200 -0.57574700
H 2.62364100 2.35052700 -0.87629500
O -3.59391200 0.91570900 1.41707600
H -3.37754600 0.03586100 1.76342700
H -3.92656200 0.75369500 0.51975900
O -4.02241700 0.24381700 -1.30941600
H -4.80028700 0.27712800 -1.86901100
H -3.78395300 -0.70934100 -1.19439400
O -3.13611800 -2.20689400 -0.81562400
H -3.29520700 -2.37597600 0.12152000

H -2.18842600 -2.00770700 -0.83976500

$(H_2SO_4)(NH_3)(H_2O)_9$ [4-5] Cluster (1.23 kcal/mol), $\Delta\alpha = 17.22$, $\bar{\alpha} = 133.09$

S -1.09389800 -1.33721300 -0.03046500
O -0.01948400 -2.32247300 -0.06513200
O -2.33992100 -1.79017300 -0.60770900
O -1.32537400 -1.14084900 1.51636000
H -2.02263900 -0.45769500 1.63228200
O -0.67901300 -0.04589300 -0.55422100
H 1.48475700 1.11590000 -0.26008400
N 1.64473200 1.23248300 -1.29514800
H 0.88152100 1.79538500 -1.67882600
H 1.64519300 0.29862100 -1.72217100
H 2.56248600 1.68429000 -1.36524100
O 1.50110000 1.21433800 1.41908000
H 0.63001000 1.63044900 1.57222300
H 1.46136000 0.30461200 1.75075000
O -0.86242800 2.61649000 1.34343600
H -1.66058100 2.09594700 1.50222000
H -0.88415700 2.78001900 0.39051000
O -1.02104600 2.39293700 -1.55606200
H -1.75395100 2.74008100 -2.06718900
H -1.26769500 1.47999100 -1.32230000
O 1.80679900 -1.59650700 -1.97115400
H 1.13197300 -1.94606200 -1.35429800
H 1.77062400 -2.14745700 -2.75477700
O -3.55863600 0.53975300 -1.28098800
H -4.40889200 0.44684000 -1.71447800
H -3.17910600 -0.36304300 -1.22297000
O -3.16079400 0.86899600 1.38701700
H -3.96471000 0.92163900 1.90727700
H -3.42989600 0.83253800 0.44330700
O 3.77817900 -0.81123200 -0.05252000
H 3.33550800 -1.24015500 -0.79547800
H 3.28943000 -1.11207100 0.72618300
O 4.04415400 1.98555000 -0.05287300
H 3.48423300 2.13698200 0.71707700
H 4.18401200 1.02408900 -0.02910600
O 1.81342300 -1.56970900 1.87259200
H 1.13673200 -1.96956700 1.29604400
H 1.74736200 -2.01312100 2.71990900

$(H_2SO_4)(NH_3)(H_2O)_9$ [5-4] Cluster (0.00 kcal/mol), $\Delta\alpha = 27.34$, $\bar{\alpha} = 135.38$

S -0.18975900 0.00436500 0.18796500
O 1.12031500 0.45009600 0.69205800
O -1.18410600 -0.03632200 1.27276600
O -0.63671800 0.96549200 -0.85286400
H -1.93612800 0.62705400 -1.44924700
O -0.05135800 -1.34737800 -0.40777900
H 1.55361300 -1.71891400 -0.62775800
N 2.59394200 -1.87102300 -0.63378000
H 2.83060200 -2.73226400 -1.11329100
H 2.89895700 -1.90595600 0.34381700

H 3.08233600 -1.02998500 -1.09617500
O -2.86162800 0.29393600 -1.78547300
H -3.55677100 0.58353000 -1.06783400
H -2.79654600 -0.72316900 -1.72065200
O -3.44208600 -1.47460200 1.24373300
H -3.60921800 -1.92891900 2.07114900
H -2.57412200 -1.01983700 1.33769500
O 2.00809600 2.19842300 -1.33794600
H 1.19303900 2.14317600 -1.84588900
H 1.74464200 1.79874200 -0.49378400
O -2.51604100 -2.19227500 -1.32092800
H -2.99009700 -2.28548400 -0.48033800
H -1.58262400 -2.09598100 -1.05073300
O -2.52426600 2.40911200 1.31262000
H -1.96061900 1.62337000 1.42978200
H -2.03394400 2.96178800 0.69922000
O -4.41907600 0.90924200 0.08425000
H -3.88431700 1.57022100 0.57625500
H -4.38006400 0.10472100 0.62584300
O 2.98411200 -0.83842700 2.00738100
H 2.20591100 -0.33020700 1.67260400
H 2.82167000 -1.03018300 2.93218100
O 5.18833200 0.40793700 0.81335600
H 5.44508000 1.25100900 1.19019500
H 4.48279500 0.05904100 1.38257800
O 3.86158000 0.21786500 -1.63408200
H 3.24281300 0.97573600 -1.68412700
H 4.46430100 0.42502000 -0.89921300

$(H_2SO_4)(NH_3)(H_2O)_9$ [6-3] Cluster (4.14 kcal/mol), $\Delta\alpha = 23.19$, $\bar{\alpha} = 135.35$

S 0.46240800 0.11668200 -0.11713900
O 1.66302700 0.02759900 -0.93377800
O -0.78136900 0.05620400 -0.84683100
O 0.52436100 -1.14990700 0.79294600
H -0.42078600 -1.43921500 1.12599000
O 0.53185200 1.28588300 0.76835200
H 2.29276100 1.70600300 0.91071500
N 3.30779800 1.50833100 0.96997800
H 3.38037800 0.53189000 1.35962900
H 3.78594800 2.18192500 1.55728100
H 3.70762300 1.48754600 0.00495900
O -1.75051900 -1.86957600 1.51503100
H -1.83391600 -2.29600100 2.37015500
H -2.44422500 -1.10483300 1.48062900
O -2.46242300 -2.23291300 -1.32117400
H -2.37649600 -2.53356400 -0.41002300
H -1.80619100 -1.52552900 -1.37533700
O -1.99977300 2.39904900 1.12553300
H -1.08389400 2.08426800 1.01860300
H -1.98770800 3.04935400 1.82935600
O -4.58496100 -0.35369300 -0.99473500
H -4.01722100 -1.08548400 -1.28586600
H -4.18416300 0.44119500 -1.38394100

O -3.44606600 -0.02546900 1.39211900
H -3.01410300 0.84075200 1.32736600
H -3.95893000 -0.13904800 0.55118700
O -2.91097200 1.85228900 -1.57967100
H -2.85374700 2.34802800 -0.75479000
H -2.11811100 1.30130000 -1.54642700
O 3.76854900 -1.64354100 -1.00983200
H 3.76200500 -2.46680700 -1.50174000
H 2.87459200 -1.25649900 -1.08407700
O 3.25964700 -1.10672000 1.70977700
H 2.31028800 -1.28825000 1.64783300
H 3.62589200 -1.52828100 0.91657700
O 4.19586400 1.13262900 -1.63048900
H 4.45115200 0.19977700 -1.58916300
H 3.29800900 1.09158700 -1.98250800

$(H_2SO_4)(NH_3)(H_2O)_9$ [7-2] Cluster (4.12 kcal/mol), $\Delta\alpha = 24.62$, $\bar{\alpha} = 134.92$

S 0.69116500 0.02602500 -0.15345500
O 1.58429600 -0.72032200 -1.05552100
O -0.70284300 -0.03312700 -0.65574400
O 0.74611800 -0.52333400 1.20773500
H -0.72845700 -1.06136700 1.81575300
O 1.11879500 1.45969100 -0.12824900
H 2.55606900 1.53996100 -0.69981600
N 3.48843000 1.28918900 -1.17690300
H 3.86247400 2.04667700 -1.73592700
H 3.23010100 0.48950400 -1.75767200
H 4.17919100 0.96173700 -0.45990900
O -1.65968900 -1.20988300 2.10344300
H -2.07415300 -1.71756800 1.38506900
H -2.21699600 0.08868700 2.00646100
O -1.02599100 -2.37987500 -2.00983200
H -0.21354200 -2.88453600 -1.93044800
H -0.78280100 -1.48694600 -1.69943700
O -2.69220300 1.01848800 1.81523200
H -3.27445600 0.81991700 1.00039100
H -2.00684500 1.71210200 1.51558900
O -2.10412700 1.97042700 -1.63846100
H -1.94988500 2.19689800 -2.55658600
H -1.46566100 1.25666100 -1.40010400
O -3.96354600 0.36269600 -0.29598000
H -3.66011200 -0.55541000 -0.40664500
H -3.50945100 0.88616000 -0.97604000
O -1.09663400 2.78968700 0.88300700
H -1.48995300 2.90662700 0.00541600
H -0.21799400 2.41529300 0.68246400
O -2.96925900 -2.28095000 -0.17185800
H -2.27637800 -2.46146700 -0.84866000
H -3.57852400 -3.02109300 -0.19045000
O 3.25376000 -1.78718900 0.95157700
H 2.53624400 -1.46366600 1.51520900
H 2.82007800 -1.73208500 0.08529300
O 5.11054900 0.07276800 0.62499300

H 4.48944400 -0.66512600 0.85483500
H 5.50014100 0.37570300 1.44609000

$(H_2SO_4)(NH_3)(H_2O)_9$ [8-1] Cluster (10.09 kcal/mol), $\Delta\alpha = 25.40$, $\bar{\alpha} = 135.23$

S 1.25034500 -0.61265500 -0.74077200
O 2.27854700 -1.55523100 -1.13003000
O 0.13358600 -0.52235300 -1.66784800
O 0.71474700 -1.01402100 0.62786000
H 0.30931200 0.15266400 1.40295700
O 1.85956700 0.74685000 -0.54345600
H 3.29024900 0.45048600 -0.15523000
N 4.22035800 -0.06914100 0.08663700
H 4.95369500 0.53889300 0.43094800
H 4.49678100 -0.54481300 -0.76868100
H 3.95264200 -0.80581900 0.78046100
O -0.07057300 0.95102200 1.95260800
H -1.08481400 1.01865100 1.73080300
H 0.34208500 1.82999900 1.64605300
O -3.78054900 -1.14743700 -1.33788200
H -2.98153200 -1.53996900 -0.90805000
H -4.06954700 -1.77166700 -2.00542900
O 0.77069600 3.20804300 1.11498800
H 0.30531100 3.96442600 1.47691600
H 0.55216500 3.17381100 0.14576500
O -1.99185000 1.04655600 -1.39913200
H -2.75320200 0.54435100 -1.71836500
H -1.22974200 0.42767700 -1.49565200
O -2.43626300 1.21552800 1.23162400
H -3.11924900 0.55466000 1.43199200
H -2.32571600 1.19510900 0.24954800
O 0.25018700 2.83962200 -1.44449600
H -0.63269400 2.49430800 -1.63272700
H 0.82958100 2.05951600 -1.45254600
O -1.89223900 -2.05352700 0.26613900
H -2.30101600 -1.87380800 1.11791100
H -0.96955800 -1.75108900 0.32378100
O -4.30219700 -0.86244600 1.36273600
H -5.17401200 -0.84295300 1.75972700
H -4.42599300 -0.98411300 0.40467700
O 3.10229800 -2.03026000 1.69565900
H 2.19366100 -1.74874900 1.47292800
H 3.20593300 -2.83384500 1.17795300

$(H_2SO_4)(NH_3)(H_2O)_9$ [9-0] Cluster (7.58 kcal/mol), $\Delta\alpha = 22.12$, $\bar{\alpha} = 136.76$

S -2.54019800 0.18769300 0.00041800
O -3.95983300 0.18400000 -0.14122100
O -1.76310900 1.12529500 -0.75728200
O -2.19292000 0.30659000 1.47198300
H -1.20652600 0.72861100 1.65024700
O -2.00839100 -1.21780200 -0.41879000
H -2.74139100 -1.93253900 -0.24776700
N -4.03985000 -2.77864700 0.02398100
H -4.31333600 -3.44999200 -0.68255500

H -4.71459400 -2.01794300 0.02384400
H -4.08073000 -3.23600000 0.92653600
O -0.01055900 1.31355000 1.87018500
H 0.67600200 0.77369600 2.30631000
H 0.39134800 1.62448000 1.02494200
O -0.66775200 3.47977900 -1.73240000
H -0.99107200 4.29562900 -1.34713400
H -1.30284700 2.79456000 -1.47656500
O 0.77421200 -0.77898000 -0.99421800
H -0.16073200 -1.00419600 -1.08233400
H 1.26496600 -1.11971400 -1.76569100
O 1.20323800 1.89837100 -0.45644700
H 0.69614200 2.56610200 -0.95326500
H 0.97027600 1.03011700 -0.83447600
O 2.31341000 -2.01016900 0.97713600
H 1.67590500 -1.66326400 0.32611800
H 3.16949700 -1.91840500 0.53499000
O 2.72396400 -1.58407600 -2.70029700
H 3.42245800 -1.37226700 -2.05405200
H 2.87236900 -2.49318200 -2.96416500
O 2.16187300 -0.10419100 2.77451200
H 2.33129800 -0.37850600 3.67678700
H 2.22866200 -0.90876300 2.19486900
O 4.43283300 -0.96525400 -0.60282600
H 5.38902400 -0.95560200 -0.66740600
H 4.16939400 -0.11220200 -0.16204800
O 3.62224200 1.18675400 0.66768500
H 2.87750100 1.61368300 0.20990800
H 3.26484000 0.91221500 1.52418200

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [0-10] Cluster (5.01 kcal/mol), $\Delta\alpha = 13.07$, $\bar{\alpha} = 144.75$

S 2.71094400 -0.37409500 -0.26658000
O 1.40986300 -0.74839000 -0.81093000
O 3.82619300 -1.13744500 -0.71849300
O 2.89053200 1.10333600 -0.90273700
H 3.83154500 1.30623700 -0.95078100
O 2.64478900 -0.15361100 1.16937800
H -0.16240600 -1.23793600 2.00242900
N -0.58736900 -1.30173700 1.06527500
H -1.34498100 -0.60737900 0.94217600
H -0.94516700 -2.24117400 0.87217700
H 0.15520200 -1.06677900 0.37975700
O 0.20300200 2.15784000 -1.24629700
H 1.11308300 1.87698700 -1.40298700
H -0.37008900 1.52960700 -1.72176400
O 0.22260600 1.39031800 1.48383600
H 0.19163300 1.67371800 0.55433000
H 1.12011900 1.05230700 1.60286000
O -2.71933500 0.39581800 0.27364700
H -2.66022500 1.25838700 0.75808000
H -2.47177600 0.56287400 -0.65095800
O -1.66051300 0.42442100 -2.30608200
H -2.10391300 0.60398000 -3.13682500

H -1.31769300 -0.50580200 -2.34752400
O 1.22393800 -1.35925000 3.21331900
H 1.32890900 -0.87225900 4.03191900
H 1.91660700 -1.03320100 2.61442700
O -0.63605600 -1.99648700 -2.24037500
H 0.25604700 -1.82752000 -1.90549300
H -1.06044700 -2.62162000 -1.63387600
O -2.26578900 2.62855400 1.63344700
H -1.39577200 2.34442200 1.94907300
H -2.06402300 3.34582700 1.00864200
O -1.98867200 -3.47228100 -0.21622500
H -2.85550600 -3.04181400 -0.04713000
H -2.13475100 -4.41921800 -0.23358800
O -1.32701800 4.31585600 -0.39375400
H -0.67629800 3.69943500 -0.76847700
H -0.86255300 5.14007600 -0.24309500
O -4.09551200 -1.90661000 0.29585800
H -4.82274000 -1.96824400 0.91571000
H -3.75254100 -0.98978600 0.34254200

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [1-9] Cluster (6.72 kcal/mol), $\Delta\alpha = 24.80$, $\bar{\alpha} = 144.98$

S 2.87697900 -0.04078500 -0.17803200
O 1.97633200 -1.00670100 -0.79643900
O 4.26815900 -0.21204500 -0.48102400
O 2.41525900 1.32553000 -0.87185800
H 3.02727700 2.02037200 -0.54172100
O 2.59919300 0.12686300 1.24369800
H 0.98430500 -0.56765700 1.63257800
N 0.03341700 -0.90227500 1.38845500
H -0.61268400 -0.95291500 2.19044700
H 0.13971500 -1.82728500 0.95953000
H -0.30863200 -0.21726500 0.69344400
O -0.41808400 1.23745000 -0.41514200
H -0.84814900 2.09936400 -0.22539400
H 0.48263000 1.40741000 -0.72651200
O -1.96423200 3.37863100 -0.00198800
H -1.92966000 4.07771800 0.65135500
H -2.83449200 2.93670100 0.09967600
O 4.48173800 2.50863900 0.46024700
H 4.97068200 1.73116600 0.15610200
H 4.18095000 2.25379100 1.33851700
O 1.11304600 -3.35584100 0.17708400
H 1.74425100 -2.68922600 -0.15055300
H 1.62228200 -4.08818800 0.52725700
O -2.11525400 -1.24481100 3.16817500
H -2.82719100 -1.15192300 2.50932300
H -2.42163700 -0.81834300 3.96927000
O -3.71230500 -0.83157400 0.97956500
H -3.14534200 -0.84666900 0.17611000
H -4.57626300 -1.12566200 0.67760700
O -4.22051500 1.92526100 0.26826400
H -4.02715400 1.13194400 0.78511800
H -4.59173200 1.55544200 -0.54660200

O -0.24708500 -2.24446100 -2.06008000
H 0.52075900 -1.66077500 -1.97930500
H -0.01666500 -2.98856800 -1.49073900
O -2.23026700 -0.61544000 -1.26479100
H -1.64708100 0.15733900 -1.14333800
H -1.62725200 -1.31183100 -1.60520800
O -4.86264000 0.01677500 -1.70845500
H -3.92879500 -0.23019700 -1.82650700
H -5.26246800 0.00753900 -2.57917100

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [2-8] Cluster (0.00 kcal/mol), $\Delta\alpha = 28.03$, $\bar{\alpha} = 143.07$

S -1.98660500 -1.16780500 0.02356800
O -0.95839300 -2.19746400 0.00939100
O -3.28152100 -1.60974100 0.47321200
O -1.43004900 -0.14435700 1.10178300
H -2.10016300 0.56461300 1.24913400
O -2.03726700 -0.42639900 -1.23636500
H 0.29779100 -1.52441400 -1.16121200
N 0.76916000 -0.79387300 -1.71629000
H 0.24851000 -0.67150100 -2.57940500
H 1.78087000 -0.99369400 -1.87902700
H 0.71679200 0.08694600 -1.16570700
O 0.86738500 1.70573800 -0.41837900
H -0.03099500 2.06662900 -0.61114900
H 0.94810700 1.61653200 0.54788100
O -1.64316300 2.30937200 -1.06595700
H -2.19926100 2.55780500 -0.31700600
H -1.86706300 1.37264800 -1.21651100
O -4.91480000 0.39031100 -0.49493800
H -4.54954400 0.47766100 -1.38023900
H -4.56016200 -0.46433500 -0.18697400
O 3.97848900 -1.78446300 0.69842500
H 4.37720800 -2.55450700 1.10576300
H 3.02240200 -1.77937300 0.93827800
O -3.35466300 1.77213500 1.14173500
H -3.81271400 2.05364000 1.93557500
H -4.02900600 1.33623800 0.55885000
O 3.50423700 -0.90684800 -1.92294600
H 3.67052900 0.04352000 -1.83717200
H 3.83985700 -1.30733000 -1.10501400
O 3.37752900 1.87821900 -1.33882700
H 2.43446700 1.98071000 -1.08458600
H 3.64583000 2.68703600 -1.77740900
O 4.10949500 0.97984000 1.25603700
H 4.05163800 1.35353700 0.36388600
H 4.26713700 0.03054700 1.13479000
O 1.42285200 -1.34861300 1.16680000
H 1.25019800 -0.53209400 1.65916900
H 0.56619700 -1.77856900 1.02296400
O 1.64494500 1.22803200 2.18288700
H 1.54266400 1.65519000 3.03382400
H 2.60966200 1.19846700 1.96537800

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [3-7] Cluster (2.22 kcal/mol), $\Delta\alpha = 29.53$, $\bar{\alpha} = 144.24$

S 1.36072000 0.54293100 -0.18105000
O 0.01880000 1.08112400 -0.37161200
O 1.81708100 -0.24199800 -1.31882000
O 2.26466500 1.78923300 -0.05275000
H 3.24440400 1.53531900 0.01558500
O 1.44988400 -0.21049300 1.07064800
H -0.23281700 -0.97361600 1.26379300
N -1.14734400 -1.26394100 0.88498300
H -0.99852200 -1.52711100 -0.10929600
H -1.81573200 -0.47255300 0.92762600
H -1.57020400 -2.03515000 1.40002900
O -3.29045800 0.47424200 1.44467800
H -3.79663100 -0.32209100 1.65994100
H -3.78143300 0.96491400 0.76930900
O -3.73627400 -2.29803600 1.59676700
H -4.39693000 -2.91666100 1.91156300
H -3.72648100 -2.35706300 0.61803600
O 4.40889500 -1.35886900 -0.83957400
H 4.27244000 -1.69789300 0.06126400
H 3.51518400 -1.19662000 -1.17612900
O -2.31302000 0.35148500 -1.68872500
H -1.48096000 0.66193300 -1.29108200
H -2.93600300 1.08678100 -1.58336800
O 4.72522000 1.05972500 0.11322400
H 5.36065700 1.61426700 -0.34352900
H 4.73758300 0.16690200 -0.33015300
O 3.88771400 -1.35607500 1.91285500
H 3.01622600 -0.96485600 1.74274600
H 4.45686000 -0.60079600 2.08426000
O -0.47805400 -1.78422400 -1.83750800
H 0.42730100 -1.42819300 -1.82413200
H -0.97513900 -1.14197700 -2.35789600
O -3.32642400 -2.11101800 -1.04994700
H -2.72563300 -2.69578600 -1.51964600
H -3.03862300 -1.20607500 -1.28831200
O -1.69848200 2.86574100 0.93292800
H -0.93592400 2.42415500 0.52527200
H -1.96550000 2.27436500 1.64489200
O -3.84172500 2.37815300 -0.56535100
H -3.06686700 2.75566100 -0.08638200
H -4.42994100 3.10091400 -0.78699300

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [4-6] Cluster (4.36 kcal/mol), $\Delta\alpha = 29.45$, $\bar{\alpha} = 144.37$

S -0.97021400 0.44346000 0.57495900
O 0.00631500 1.52346300 0.55001800
O -2.23624400 0.82834400 1.17580200
O -1.25296600 0.15457000 -0.93949100
H -1.90565900 -0.66895400 -0.99515900
O -0.44733600 -0.78860500 1.14673200
H 1.20051500 -1.17303900 0.84510300
N 2.21690800 -1.16804300 0.61529200
H 2.79213100 -1.33611100 1.43802000

H 2.43043800 -0.22526500 0.27218800
H 2.45282500 -1.82620700 -0.16198500
O -2.79500000 -1.80069500 -0.92529500
H -2.73110800 -2.13619100 -0.02003400
H -3.73403800 -1.48920500 -0.97315300
O -4.03968400 1.71084100 -0.81867600
H -3.45579600 1.66150600 -1.57917600
H -3.45025800 1.56841100 -0.06116700
O 1.46519000 -0.08822100 -1.94326600
H 0.51226700 -0.14181000 -1.78772100
H 1.62537500 0.85523100 -2.07741600
O -5.25373700 -0.80870700 -0.62217000
H -5.03763400 0.13557300 -0.71373100
H -5.19060900 -0.98870900 0.32469100
O 2.73318300 1.74692000 0.84124300
H 1.78003500 1.72982900 1.03228400
H 2.78362900 2.25162700 0.01974200
O -3.74713700 -1.44947300 1.75317200
H -3.21358700 -0.63599600 1.72537500
H -3.69785000 -1.76927400 2.65511300
O 4.45060300 0.03984300 2.02359300
H 3.93796200 0.81870700 1.73216500
H 4.93324000 0.29345400 2.81159300
O 3.05861000 -2.40484300 -1.68084600
H 2.58819900 -1.70312600 -2.15493600
H 3.94023300 -2.04282100 -1.51401200
O 1.42180200 2.71030300 -1.47637400
H 0.70513300 2.44023800 -0.87426000
H 1.12095500 3.49629700 -1.93487900
O 5.19096700 -0.96262300 -0.47671100
H 6.05225400 -0.70219800 -0.80580400
H 5.12988300 -0.61996400 0.42894400

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [5-5] Cluster (2.91 kcal/mol), $\Delta\alpha = 32.60$, $\bar{\alpha} = 144.31$

S -0.18214500 -0.77396200 -0.28395000
O 1.05803600 -1.54148000 -0.41747300
O -1.31051200 -1.38570700 -0.94408200
O -0.46145500 -0.81171100 1.26256200
H -1.41915500 -0.49190200 1.44676400
O 0.00904500 0.61972100 -0.65348700
H 1.71649100 2.41208400 -0.57100500
N 2.48550600 1.78286100 -0.36310600
H 3.39615500 2.26036900 -0.28823400
H 2.52675600 1.07235800 -1.10757400
H 2.26994800 1.29768100 0.54607300
O -2.85348300 0.02592000 1.52676800
H -3.38790000 -0.70059800 1.16617100
H -2.81774300 0.69154500 0.79689500
O -3.84868300 -1.93885900 -0.20081600
H -4.08590300 -2.86702000 -0.18041300
H -2.93554500 -1.88311800 -0.54442900
O 2.97103400 -1.93810700 1.47031100
H 3.00741800 -2.79241300 1.90287200

H 2.22057600 -1.96145200 0.84414700
O -2.62003500 1.71859500 -0.55510900
H -3.26626200 1.27420700 -1.13716900
H -1.73276300 1.46330600 -0.84684200
O -5.06349300 2.09686400 0.96818200
H -4.71993700 1.56288200 1.69075100
H -4.27450700 2.49471200 0.58145400
O -4.88869300 0.44953700 -1.40718800
H -5.28048300 0.89379900 -0.64145200
H -4.73861200 -0.46197200 -1.12327500
O 2.78917100 -0.46549100 -2.16390600
H 2.10346400 -0.96771500 -1.67587900
H 2.61722000 -0.58880500 -3.09878800
O 4.72977300 -0.38112200 -0.11505300
H 4.30434600 -0.97928300 0.51605100
H 4.31337200 -0.57634300 -0.96512400
O 1.92189400 0.59932000 2.03117900
H 2.42754100 -0.22186700 2.12238300
H 1.00439200 0.29438500 1.99046400
O 5.21013000 2.28605900 -0.14589700
H 5.86431000 2.68961100 0.42486100
H 5.26078200 1.32058200 -0.01170500

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [6-4] Cluster (1.09 kcal/mol), $\Delta\alpha = 25.90$, $\bar{\alpha} = 143.60$

S 0.11932500 -0.17201800 -0.67130100
O -0.96086700 0.62845500 -1.25300800
O 1.41258400 0.12069500 -1.28416900
O 0.20599100 0.20047800 0.80478200
H 1.38514000 -0.45888700 1.41455400
O -0.20177200 -1.60459500 -0.75467600
H -2.08592900 -1.67267900 -0.99335300
N -3.00949500 -1.31240500 -0.70946000
H -3.68082800 -2.05247100 -0.52027200
H -3.35160900 -0.61021200 -1.39008700
H -2.84640500 -0.81319800 0.18681900
O 2.22705200 -0.97923700 1.71699900
H 3.01630300 -0.40825300 1.47754500
H 2.23193500 -1.84408300 1.08485300
O 0.21365100 2.92667600 1.25320000
H 0.29646000 3.10847600 2.19147800
H 0.16792700 1.95401800 1.16939200
O 2.15407200 -2.85289800 0.11440600
H 1.29490900 -2.66307000 -0.30776200
H 2.82989600 -2.53139100 -0.52252100
O 2.63095200 2.36435300 -0.23730400
H 1.93756000 2.80055600 0.27878100
H 2.15326800 1.71589600 -0.78630800
O 4.13268200 0.56936600 0.87966500
H 4.86193400 0.91552400 1.39660100
H 3.62429600 1.34687000 0.50330400
O 3.80878300 -1.32640800 -1.38750200
H 4.27579200 -0.76512000 -0.75733900
H 3.02160000 -0.80451200 -1.61098400

O -2.49173100 2.32993800 0.17444900
H -1.84780300 1.80135200 -0.33984000
H -1.95857900 3.04707600 0.53409800
O -2.45570900 0.03087100 1.71800800
H -2.64164500 0.93439100 1.40222700
H -1.48995700 -0.04101100 1.62891100
O -3.56109100 0.98602400 -2.24607400
H -3.70675700 1.67817000 -1.58908900
H -2.61229900 1.04574000 -2.42024100
O -4.27160100 -2.11840900 1.65744000
H -4.72876300 -2.53613200 2.38796800
H -3.73315800 -1.41040800 2.03855000

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [7-3] Cluster (4.86 kcal/mol), $\Delta\alpha = 29.13$, $\bar{\alpha} = 145.74$

S 0.42784700 -0.12354700 -0.41105800
O 1.57775600 -0.40557200 -1.25823000
O -0.83617600 -0.07659900 -1.12023300
O 0.36754000 -1.29087700 0.59410100
H -0.59726500 -1.41020400 1.05581900
O 0.65227600 1.11148800 0.36411700
H 2.26275400 1.53517700 0.22883300
N 3.26268100 1.44275600 -0.08036600
H 3.78805100 2.30957000 -0.13150300
H 3.21553800 1.01014800 -1.00454000
H 3.77043800 0.77967700 0.52930400
O -1.80145500 -1.64093400 1.66478600
H -2.31180200 -0.83177100 1.86758000
H -2.37798000 -2.23174000 1.12688600
O -2.97336900 -1.68479700 -2.14777800
H -3.50126300 -0.90885700 -1.91326100
H -2.06799400 -1.36378200 -2.03321900
O -1.53107200 2.58974500 1.32578600
H -0.74948100 2.14198200 0.96452900
H -1.94241000 3.06948800 0.58608700
O -3.44377700 0.80306500 -0.76940100
H -2.49148400 0.60077000 -0.77574200
H -3.70439100 0.67797300 0.15456400
O -3.17130400 0.69297500 2.04501300
H -3.63525700 0.88722100 2.86050900
H -2.55644500 1.45741200 1.86032200
O -3.06691000 3.54198400 -0.79295000
H -3.33240500 2.61784800 -0.95356200
H -2.80143200 3.89712400 -1.64197600
O -3.33523200 -3.14921500 0.07775900
H -3.23533700 -2.71651400 -0.79992800
H -3.18021000 -4.08509400 -0.05519300
O 3.00742400 -2.36016300 0.11088400
H 2.26041000 -2.48652500 0.70666900
H 2.59633500 -1.83257900 -0.59631900
O 4.77111000 -0.65815800 1.05286800
H 4.16238800 -1.38636200 0.75215300
H 5.06116900 -0.88005400 1.93893000
O 5.91707000 1.20890300 -0.68207400

H 5.85770600 0.39643200 -0.15970300
H 6.75501500 1.17534600 -1.14492200

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [8-2] Cluster (6.48 kcal/mol), $\Delta\alpha = 34.01$, $\bar{\alpha} = 144.67$

S 1.43358600 -0.15538100 -0.72677900
O 2.71335600 -0.74881900 -1.04079400
O 0.36697600 -0.44627600 -1.65077900
O 1.05038100 -0.80968400 0.65051200
H 0.08073300 -0.58668700 0.89219300
O 1.56550300 1.28829200 -0.46329000
H 3.00669700 1.57281500 0.22423100
N 3.92289200 1.51548800 0.75559100
H 4.13065700 2.37999100 1.24213500
H 4.67809000 1.25169200 0.11753900
H 3.82207400 0.70009900 1.41367700
O -1.38541600 -0.26571300 1.13743200
H -1.84329100 -1.09241300 1.39357200
H -1.75376000 -0.00389800 0.26652900
O -1.80098900 -2.23530300 -1.25509800
H -1.71372800 -2.74503300 -0.44246700
H -0.93859500 -1.82338600 -1.40778800
O -0.77022800 2.92429700 -0.54420400
H 0.09098200 2.49482500 -0.44040400
H -1.19360700 2.92666500 0.33221600
O -2.21689300 0.85184300 -1.27481200
H -1.74113300 0.29284600 -1.89740700
H -1.65079500 1.65828300 -1.14398800
O -4.31866000 -1.48843200 -0.23261800
H -4.54675100 -0.55802800 -0.09742800
H -3.58437600 -1.50273700 -0.86624500
O -2.38220500 2.38548600 1.69291600
H -3.23839400 2.22563000 1.27283500
H -2.03695500 1.49761600 1.85246900
O -2.69011000 -2.63268500 1.49819100
H -3.01314000 -3.08719100 2.27677100
H -3.47045400 -2.30213000 0.99362300
O -4.52803400 1.37908400 -0.05132600
H -5.23759300 1.86925800 -0.47041800
H -3.81266600 1.28875900 -0.71012900
O 3.61356300 -0.88108100 1.98016600
H 2.72598600 -1.11381800 1.66846200
H 4.22071000 -1.32078200 1.37194200
O 5.30988900 -0.61447100 -0.40941500
H 4.43957100 -0.77186600 -0.82231800
H 5.96507200 -1.02513500 -0.97532300

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [9-1] Cluster (7.48 kcal/mol), $\Delta\alpha = 35.33$, $\bar{\alpha} = 144.63$

S -2.01471400 -0.33052000 -0.58635000
O -3.15415400 -0.27369400 -1.48115900
O -0.84057600 -0.97343500 -1.13988900
O -1.66466800 1.14453700 -0.28298000
H -0.95710000 1.25427500 0.50719500
O -2.40254300 -0.94770800 0.70572100

H -3.92123100 -0.89886100 0.77652800
N -4.97790600 -0.72294600 0.59752600
H -5.56507400 -0.96973900 1.38592500
H -5.23011700 -1.26247700 -0.22682500
H -5.04981100 0.29009100 0.34814900
O -0.05169300 1.41320800 1.56099300
H 0.13583000 0.50492500 1.92482000
H 0.77716600 1.82999900 1.28408700
O 1.95040900 2.86745800 0.16645300
H 2.90400200 2.67354300 0.24757100
H 1.85515600 3.81945900 0.11499000
O -0.01287000 -1.08901600 2.32551500
H -0.89232400 -1.26825100 1.96665700
H 0.57431000 -1.62785900 1.76519200
O 1.49372600 0.46034200 -1.18507500
H 1.33364800 1.39590400 -1.00465100
H 0.62903500 0.02947000 -1.30529100
O 2.80271900 -0.13693200 1.21043400
H 3.16358100 -1.03178200 1.15982100
H 2.21576500 -0.07919400 0.43288400
O 1.08592300 -2.60171600 0.28882400
H 1.97007800 -2.58484800 -0.10405000
H 0.47322200 -2.21989600 -0.35297000
O 4.43152300 1.74779800 0.40902700
H 5.13044200 2.00551300 1.01196600
H 3.93573500 0.99726700 0.83247300
O 3.83686500 -2.31509200 -0.29619300
H 4.38755700 -3.06275500 -0.53136400
H 4.06684400 -1.57870600 -0.90720700
O 4.16906800 -0.11584800 -1.80995000
H 4.53579000 0.57781200 -1.24641700
H 3.22315400 0.09724200 -1.85496300
O -4.69377000 1.78770000 -0.46251800
H -4.10326800 2.39772200 -0.01234300
H -4.11129600 1.31926900 -1.08689000

$(H_2SO_4)(NH_3)(H_2O)_{10}$ [10-0] Cluster (3.22 kcal/mol), $\Delta\alpha = 31.96$, $\bar{\alpha} = 145.53$

S -2.18478300 -0.03308400 -0.13378200
O -3.19104200 0.66270500 -0.89974500
O -0.91180000 -0.21670500 -0.82103500
O -1.96744500 0.60507800 1.17821400
H -0.73153900 0.19634600 1.87270200
O -2.69404900 -1.47302400 0.14064500
H -3.72057900 -1.48985200 0.11362300
N -5.30031800 -1.26594800 -0.08905800
H -5.78375400 -1.92468400 -0.68639700
H -5.24088600 -0.37522000 -0.57524900
H -5.85426800 -1.13413800 0.74791100
O 0.17466900 -0.02864000 2.31520600
H 0.86328100 0.72712500 2.03547300
H 0.50191000 -0.91580400 1.98225100
O -1.94250200 3.23022800 -0.33685400
H -2.52499600 2.66741100 -0.86375100

H -1.99518800 2.81453800 0.53166900
O 1.14518200 -2.27123200 1.42309500
H 0.88838100 -3.08055900 1.86985600
H 0.93590400 -2.39275500 0.43949600
O 0.55234600 2.12546400 -0.84062100
H -0.19092200 2.75502400 -0.79794400
H 0.09993800 1.26452000 -0.92066900
O 1.67303600 1.78367300 1.57689500
H 2.61737000 1.57603500 1.44988300
H 1.31100800 2.01899700 0.69147500
O 0.68616600 -2.43620200 -1.08951600
H 1.45502800 -2.09083500 -1.57385400
H -0.00688500 -1.76079000 -1.18284800
O 4.21180100 1.01639500 0.88501600
H 4.14063900 0.02780400 0.83971400
H 5.05608100 1.23378900 1.28224300
O 3.03241500 -1.30414800 -2.10673700
H 3.02434000 -0.31393000 -2.04777600
H 3.46219800 -1.53493200 -2.93155200
O 3.09246800 1.30650000 -1.71394000
H 3.58202200 1.40761100 -0.88449200
H 2.24298100 1.75544600 -1.58088800
O 3.80076700 -1.56368400 0.57902700
H 3.63732000 -1.65262900 -0.37429600
H 2.99327500 -1.87879500 1.01013100