Theoretical studies on the coupling interactions in $H_2SO_4\cdots HOO^{\bullet}\cdots(H_2O)_n$(n=0-2) clusters: Toward understanding the role of water molecules in the uptake of $HOO^{\bullet}$ radical by sulfuric acid aerosols

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Supplementary Information

1. Comparisons between B3LYP and MP2 methods

As mentioned in the section of computational methods, the MP2 method has also been used for clusters **R1** and **N1** employing the same basis set. As a result, the reliability of the B3LYP method can be confirmed through the comparisons of the geometry and binding energy with MP2 method, which is summarized as follows.

As displayed in Fig. S1, the optimized geometries for clusters **R1** and **N1** are well consistent with each other at both levels. Taking **R1** as an example, as presented in Table S1, the intermolecular H-bond distances are 1.665 and 1.704 Å for O10···H7-O6 and O2···H9-O8 at the B3LYP/6-311++G(3df,3pd) level of theory, which are larger by only 0.051 and 0.048 Å than those of MP2 results. On the other hand, the bond distance variations of the O-H bonds associated with the intermolecular H-bonds can be comparable to each other at both levels. For clusters **N1**, the same results can be also observed. Therefore, the predicted geometrical features at the B3LYP method can be comparable to the MP2 method.

As for the calculated binding energy of **R1** and **N1** according to reaction (1) in the text, B3LYP method can give well consistent results with MP2 method. For example, as presented in Table S1, the calculated value of -11.59 kcal mol^{-1} for **R1** cluster can be comparable to that of -11.55 kcal mol^{-1} at the MP2 level. In other words, only a difference of 0.04 kcal mol^{-1} has been observed for the calculated binding energy of **R1** cluster at both levels. Similarly, a small difference of 0.45 kcal mol^{-1} has been observed for the binding energy of **N1** cluster at both levels.

Therefore, the reliability and validity of the B3LYP/6-311++G(3df,3pd) level of theory employed should be confirmed for the studied systems.

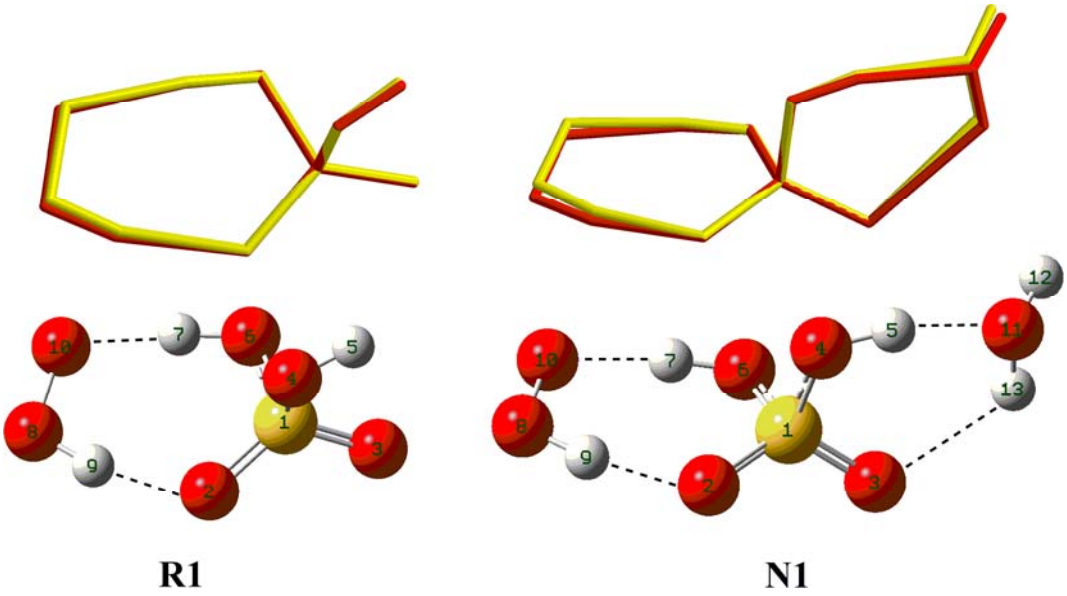

Fig. S1 The superposition of two geometries for clusters **R1** and **N1** employing the B3LYP (red color) and MP2 (yellow color) methods at the 6-311++G(3df,3pd) basis set.

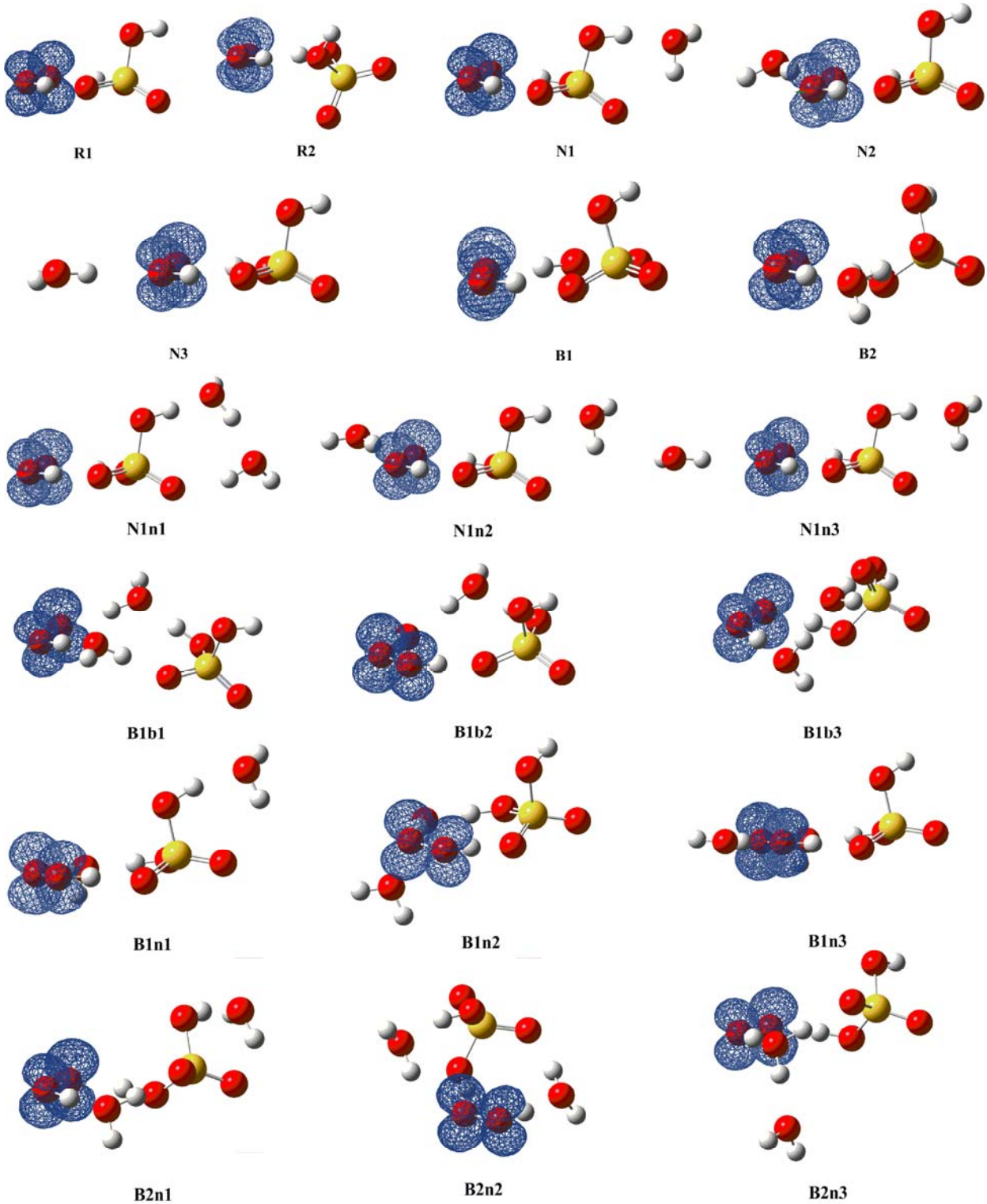

Fig. S2 Spin density maps of $H_2SO_4\cdots HOO^{\bullet}\cdots(H_2O)_n$(n=0-2) clusters. The isodensity contours are 0.003 electron bohr^{-3}.

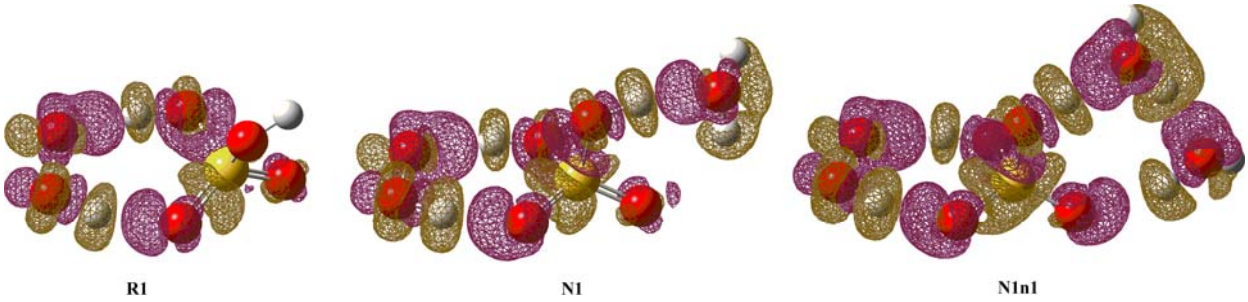

Fig. S3 Electron density difference maps for clusters **R1**, **N1**, and **N1n1**. The yellow regions represent depleted electron density and violet regions designate increased electron density. The isodensity contours are 0.002 electron bohr^{-3}.

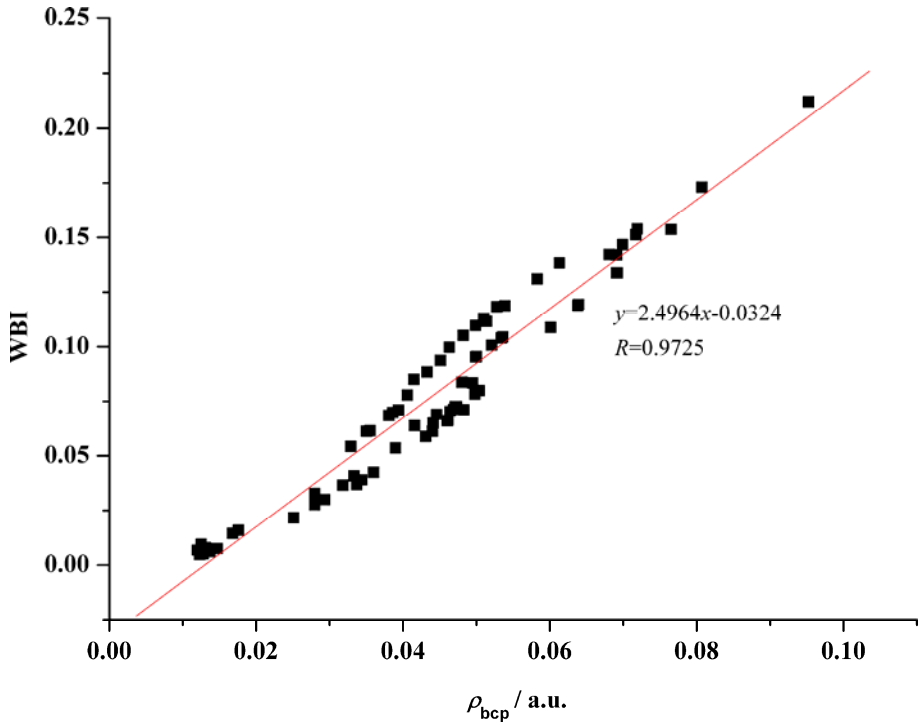

Fig. S4 The WBI as a function of the electron density at the BCP of the intermolecular H-bond.

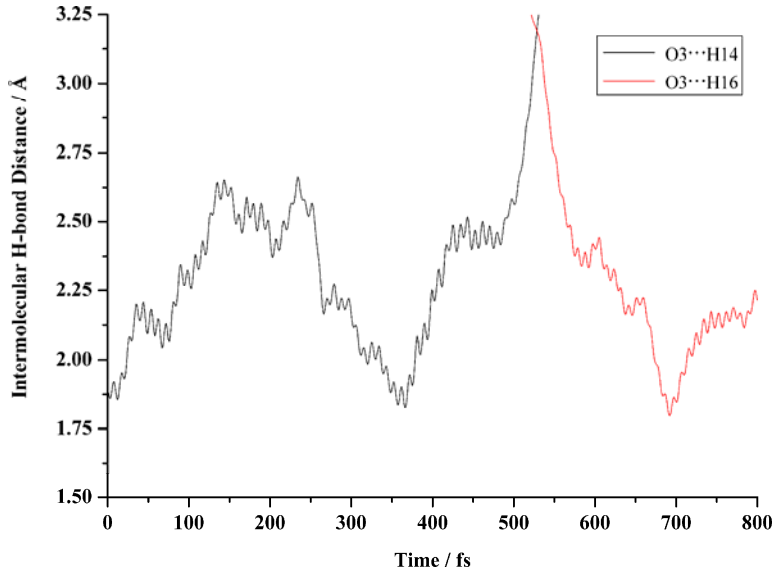

Fig. S5 The variations of H-bond distances between H_2SO_4 and the second water in **N1n1** cluster as a function of time.

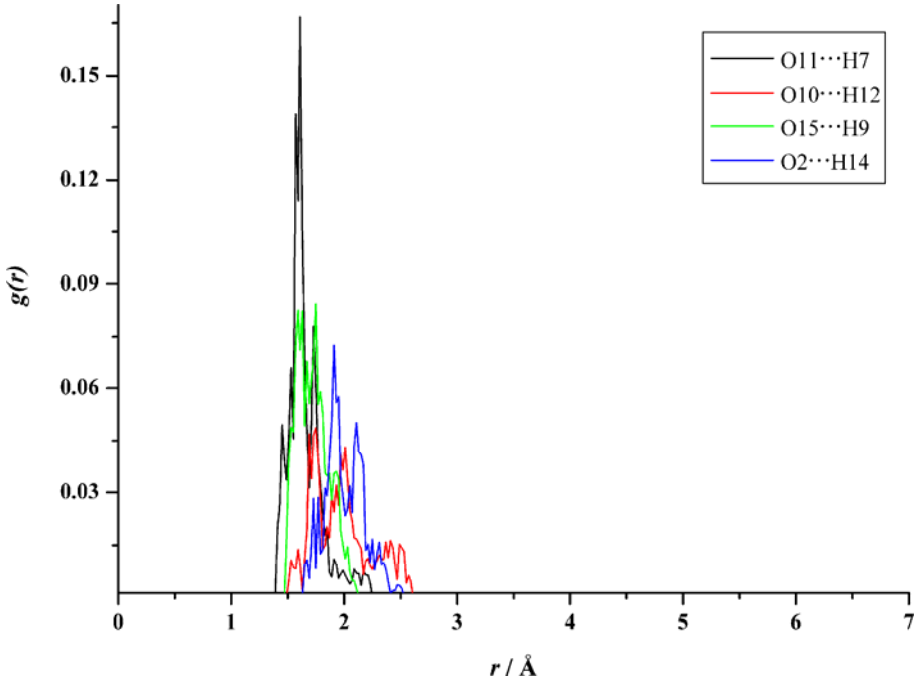

Fig. S6 Radial distribution functions for the H-bond distances in **B1b1** cluster.

Table S1 The comparison between the B3LYP and MP2 methods at the 6-311++G(3df,3pd) basis set for clusters **R1** and **N1**.

		B3LYP	MP2
The selected structure parameters			
R1	R(O10···H7-O6)[a]	1.665	1.614
	R(O2···H9-O8)	1.704	1.656
	Δr(H7-O6)[b]	0.037	0.040
	Δr(H9-O8)	0.023	0.026
N1	R(O10···H7-O6)	1.679	1.631
	R(O2···H9-O8)	1.684	1.643
	R(O11···H5-O4)	1.652	1.638
	R(O3···H13-O11)	2.263	2.235
	Δr(H7-O6)	0.035	0.037
	Δr(H9-O8)	0.024	0.028
	Δr(H5-O4)	0.034	0.032
	Δr(H13-O11)	0.007	0.007
The calculated binding energy for the reaction:			
$H_2SO_4 + HOO^{\bullet} + nH_2O \rightarrow H_2SO_4\cdots HOO^{\bullet}\cdots(H_2O)_n(n=0\text{-}1)$[c]			
R1		-11.59(1.97)[0.90]	-11.55(2.23)[2.96]
N1		-20.56(4.23)[1.48]	-21.01(4.53)[4.64]

[a] R refers to the H-bond length (in angstroms).

[b] Δr refers to the changes of O-H bonds upon the formation of clusters (in angstroms).

[c] The binding energies consider BSSE and ZPVE corrections (in kcal mol^{-1}), where the data in parentheses and brackets refer to the ZPVE and BSSE corrections, respectively.

Table S2 The stretching vibrational frequencies and corresponding red-shifts of the O-H bonds involved in the intermolecular H-bonds in all the clusters [a]

Monomers/Clusters	H-bonds	ν^b	$\Delta\nu^b$
H_2SO_4	O6-H7/O5-H4	3769.3	
$HOO^\bullet$	O-H	3604.2	
H_2O	O-H	3815.7(3914.8)	
$H_2SO_4\cdots HOO^\bullet$			
R1	O10···H7-O6	3013.7(3239.4)*	-755.7(-530.0)
	O2···H9-O8	3013.7(3239.4)*	-590.5(-364.8)
R2	O10···H7-O6	3256.2	-513.1
	O4···H9-O8	3431.4	-172.8
$H_2SO_4\cdots HOO^\bullet\cdots H_2O$			
N1	O10···H7-O6	3047.1(3217.6)*	-722.2(-551.7)
	O2···H9-O8	3047.1(3217.6)*	-557.0(-386.6)
	O11···H5-O4	3093.2	-676.2
	O3···H13-O11	3749.9	-65.8
N2	O10···H7-O6	3119.2(3238.9)*	-650.2(-530.5)
	O2···H9-O8	3119.2(3238.9)*	-485.0(-365.3)
	O10···H12-O11	3775.5	-40.2
N3	O10···H7-O6	3078.1(3209.6)*	-691.3(-559.8)
	O2···H9-O8	3078.1(3209.6)*	-526.1(-394.6)
	O8···H12-O11	3805.7	-10.0
B1	O11···H7-O6	2662.8	-1106.5
	O10···H12-O11	3429.9	-385.8
	O2···H9-O8	3262.7	-341.5
B2	O10···H7-O6	3037.2	-732.1
	O11···H9-O8	2850.0	-754.2
	O2···H13-O11	3556.2	-259.5
$H_2SO_4\cdots HOO^\bullet\cdots (H_2O)_2$			
N1n1	O10···H7-O6	3060.7(3206.3)*	-708.6(-563.1)
	O2···H9-O8	3060.7(3206.3)*	-543.4(-397.9)
	O11···H5-O4	2635.3	-1134.0
	O15···H13-O11	3375.9	-439.7
	O3···H14-O15	3661.9	-153.7
N1n2	O10···H7-O6	3098.5(3259.9)*	-670.9(-509.4)
	O2···H9-O8	3098.5(3259.9)*	-505.7(-344.3)
	O10···H12-O11	3767.7	-47.9
	O15···H5-O4	3063.3	-706.1
	O3···H14-O15	3758.8	-56.8
N1n3	O10···H7-O6	3072.5(3216.8)*	-696.9(-552.5)
	O2···H9-O8	3072.5(3216.8)*	-531.7(-387.4)
	O8···H12-O11	3802.7	-12.9
	O14···H5-O4	3059.9	-709.5

	O3···H16-O14	3756.9	-58.8
B1b1	O11···H7-O6	2735.9	-1033.4
	O10···H12-O11	3417.5	-398.2
	O15···H9-O8	2957.2	-647.0
	O2···H14-O15	3566.7	-249.0
B1b2	O11···H7-O6	2467.2	-1302.2
	O15···H12-O11	3235.1	-580.6
	O10···H14-O15	3526.6	-289.1
	O2···H9-O8	3286.2	-317.9
B1b3	O10···H7-O6	2706.5(2909.2)*	-1062.8(-860.2)
	O15···H9-O8	2706.5(2909.2)*	-897.7(-695.0)
	O11···H16-O15	3345.3	-470.4
	O2···H13-O11	3640.5	-175.1
B1n1	O11···H7-O6	2741.8	-1027.6
	O10···H12-O11	3436.7	-379.0
	O2···H9-O8	3231.4	-372.7
	O14···H5-O4	3132.5	-636.9
	O3···H16-O14	3739.8	-75.8
B1n2	O11···H7-O6	2122.6	-1646.8
	O15···H13-O11	3571.0	-244.6
	O10···H12-O11	3495.2	-320.5
	O2···H9-O8	3229.0	-375.1
B1n3	O11···H7-O6	2701.6	-1067.7
	O10···H12-O11	3480.7	-335.0
	O8···H14-O15	3800.0	-15.7
	O2···H9-O8	3190.7	-413.5
B2n1	O10···H7-O6	3081.4	-687.9
	O11···H9-O8	2855.6	-748.6
	O2···H13-O11	3527.6	-288.1
	O15···H5-O4	3134.3	-635.1
	O3···H14-O15	3739.7	-76.0
B2n2	O15···H5-O4	3186.1	-583.3
	O10···H14-O15	3747.1	-68.6
	O10···H7-O6	3318.6	-450.7
	O11···H9-O8	2736.4	-867.8
	O2···H13-O11	3436.0	-379.7
B2n3	O10···H7-O6	2933.1	-836.2
	O11···H9-O8	2587.1	-1017.1
	O15···H12-O11	3594.6(3649.8)	-221.1(-265.1)
	O2···H13-O11	3594.6(3649.8)	-221.1(-265.1)

[a] All the units are in cm^{-1}. The asterisk (*) refers to the significant resonant coupling between the stretching vibrational modes of O6-H7 bond of H_2SO_4 fragment and that of O8-H9 bond of $HOO^{\bullet}$ fragment.

[b] The data in parentheses refer to the asymmetric stretching vibrational frequencies.

All the Cartesian coordinates of the geometries obtained at the B3LYP/6-311++G(3df,3pd) level of theory.

1. $H_2SO_4\cdots HOO$

R1

S	0.88438500	-0.07133100	-0.11932400
O	-0.04543400	-1.15430100	-0.30647300
O	2.07084900	0.02485500	-0.89091400
O	1.27121200	-0.15192300	1.41992200
H	2.08895200	0.34197600	1.57694800
O	0.11246000	1.27493300	-0.23197100
H	-0.86866500	1.13034400	-0.06780000
O	-2.64736000	-0.60502800	-0.02465500
H	-1.73389900	-0.98620000	-0.15132200
O	-2.46629500	0.69336100	0.10301100

R2

S	0.97006200	-0.04055300	0.10446800
O	0.70289000	-0.08878200	1.49721700
O	2.27645900	0.02893800	-0.44409900
O	0.13467900	1.26884200	-0.40358800
H	0.45263600	1.52950100	-1.28035400
O	0.21062500	-1.18210900	-0.64991900
H	-0.74925900	-1.17031200	-0.39270500
O	-2.59919800	0.59070700	0.07108400
H	-1.71055200	1.00723300	-0.03008900
O	-2.41468200	-0.70729200	-0.06673700

2. $H_2SO_4\cdots HOO^{\bullet}\cdots H_2O$

N1

S	0.32112300	0.36366700	0.12028300
O	-0.74857400	1.16925600	-0.41457900
O	1.35187500	0.97456900	0.89747700
O	0.95874200	-0.38154900	-1.09102900
H	1.92049600	-0.58545500	-0.89545300
O	-0.30947900	-0.77336000	0.98394600
H	-1.26325100	-0.92593100	0.71558900
O	-3.19083600	0.11890700	-0.46815500
H	-2.34614900	0.64926800	-0.53562200
O	-2.86579600	-0.95941600	0.21533400
O	3.47225100	-0.59643200	-0.33014100
H	3.86128100	-1.39256700	0.04383600
H	3.34419500	0.02021100	0.40429900

N2

S	-1.58351700	-0.05618100	-0.08615100
O	-0.99277100	1.25603400	-0.03705800
O	-2.78297100	-0.29905100	-0.80106300
O	-1.79042100	-0.44403000	1.43867500
H	-2.41005800	-1.18495400	1.50966200
O	-0.50794900	-1.07150800	-0.57979500
H	0.40771000	-0.71897800	-0.40228700
O	1.65172400	1.45248700	0.06164600
H	0.65665500	1.55648500	0.04594000
O	1.86156100	0.16737900	-0.13178000
O	4.73546300	-0.83584900	0.09141800
H	3.88698000	-0.38608300	0.00251300
H	5.39789800	-0.17127500	-0.11374600
N3			
S	1.59670400	-0.17935900	-0.11996800
O	0.44432700	-0.99863700	-0.39272200
O	2.79221100	-0.31431100	-0.86980300
O	1.90787700	-0.44385200	1.41390600
H	2.81480000	-0.17179700	1.61683200
O	1.16281900	1.31710600	-0.15240600
H	0.17714400	1.39521400	-0.00157300
O	-1.95863300	0.07092300	-0.08549700
H	-1.14236500	-0.48994100	-0.23086300
O	-1.51499300	1.29208800	0.13124400
O	-5.04007800	-0.63584500	0.03341500
H	-4.14063600	-0.29448900	0.00466200
H	-5.60444800	0.13097300	-0.09467700
B1			
S	1.24409600	-0.16009200	-0.11822200
O	0.10140700	-0.85003100	-0.65476400
O	2.54683300	-0.42657300	-0.61500500
O	1.19471300	-0.50281100	1.43846600
H	2.04274000	-0.27877500	1.84756100
O	1.00642300	1.36295700	-0.16797700
H	0.01639300	1.61571100	-0.06830800
O	-2.45181400	-1.44901400	-0.11049800
H	-1.49107400	-1.25943400	-0.28817300
O	-3.02101600	-0.28628100	0.13110900
O	-1.45535200	1.98873600	0.08920000
H	-2.03411000	1.19331000	0.08445300
H	-1.80902500	2.59480300	-0.56823100
B2			
S	-1.31190000	0.09417800	-0.04794300
O	-0.58949800	1.22577000	0.45699300

O	-2.52998900	0.25976400	-0.75845100
O	-1.56710800	-0.80483300	1.24031600
H	-2.24944700	-1.46319800	1.04489400
O	-0.38091400	-0.78601500	-0.92891300
H	0.54149100	-0.92195400	-0.54855700
O	3.04843600	-0.64120300	0.12767700
H	2.68906700	0.30827900	0.07093700
O	2.03815000	-1.44669600	-0.11548600
O	2.06816500	1.75793900	0.06268900
H	2.20744200	2.33410700	-0.69398700
H	1.10391500	1.71810700	0.21520000

3. $H_2SO_4\cdots HOO^{\bullet}\cdots(H_2O)_2$

N1n1

S	0.11724500	-0.40695500	-0.21129600
O	1.27316800	-0.89925800	-0.91914400
O	-0.96289800	-1.30876700	0.04804300
O	-0.37365800	0.83203900	-0.98639100
H	-1.28897800	1.18080900	-0.67353700
O	0.58485600	0.14627400	1.17634500
H	1.54543700	0.42464400	1.12436100
O	3.63589100	0.08181400	-0.20435000
H	2.83141300	-0.35869200	-0.60438600
O	3.19099400	0.70302900	0.86895100
O	-2.67575300	1.67347300	-0.26914900
H	-2.70990300	2.36141000	0.40103000
H	-3.19598900	0.90672900	0.06904900
H	-2.82418800	-1.14614500	0.39798300
O	-3.69020900	-0.70934600	0.45931800
H	-4.09283700	-1.01153000	1.27724300

N1n2

S	-1.06675200	-0.41813700	0.16966100
O	-0.25844700	-1.52861000	-0.27166200
O	-2.20110100	-0.64942600	1.00288800
O	-1.50634900	0.34076900	-1.11598700
H	-2.36341400	0.83428600	-0.94324800
O	-0.13754600	0.59375700	0.91873400
H	0.80395300	0.48377100	0.61822000
O	2.34567000	-1.20246100	-0.51670000
H	1.38088200	-1.47627100	-0.49399400
O	2.37040000	-0.01083800	0.04288200
O	5.08513900	1.36013600	0.09353200
H	4.28026300	0.83045500	0.04115300
H	5.79417200	0.77009800	-0.17400800

H	-3.89301700	0.83321100	0.39942900
O	-3.82056300	1.36350200	-0.40584700
H	-3.95241700	2.28000100	-0.14484200
N1n3			
S	-1.04294500	-0.08457600	0.37425300
O	0.11548500	-0.86887600	0.72777300
O	-2.15070800	-0.01100900	1.27043500
O	-1.52517200	-0.60851000	-1.00978000
H	-2.51680300	-0.47784900	-1.09857800
O	-0.56934300	1.37771900	0.08907700
H	0.40179500	1.38743800	-0.13820800
O	2.50024400	0.00271800	0.04390800
H	1.67253300	-0.47462800	0.35101000
O	2.09076200	1.18555400	-0.36746700
O	5.56406300	-0.67428100	-0.29212100
H	4.64635800	-0.39632600	-0.20551800
H	6.05576500	0.13422000	-0.45775200
O	-4.12894300	-0.29517300	-0.86542400
H	-4.62023400	0.41355000	-1.29154400
H	-4.12339800	-0.09832400	0.08133800
B1b1			
S	1.77112100	-0.11305400	-0.22067000
O	0.67397100	-1.01497400	-0.42304600
O	2.95323800	-0.21992000	-1.00205000
O	2.15001200	-0.30342100	1.31906500
H	3.02736200	0.07143000	1.48007300
O	1.27979800	1.34946200	-0.29961600
H	0.34050400	1.48665600	0.07985300
O	-3.74843600	-0.43619600	-0.44211000
H	-2.98257800	-0.96896900	-0.04959200
O	-3.36913600	0.82433200	-0.43579500
O	-1.04307800	1.75941800	0.68709900
H	-1.84467700	1.35936200	0.28032200
H	-1.25853800	2.67673500	0.87600600
H	-0.87323600	-1.53567700	0.27737800
O	-1.76366500	-1.77673600	0.59777200
H	-1.80839600	-2.73638300	0.57613000
B1b2			
S	1.46996100	-0.23346200	-0.19181400
O	0.13565600	-0.59404000	-0.59593400
O	2.59903400	-0.72472300	-0.90135400
O	1.55215300	-0.73230900	1.32237300
H	2.47900800	-0.77701200	1.59655700
O	1.58176400	1.29549600	-0.09121800

H	0.70078700	1.75825300	0.20780200
O	-1.91834800	-2.11795400	0.22939900
H	-1.13267300	-1.57473700	-0.04639900
O	-2.95923700	-1.31034900	0.21092900
O	-0.54929900	2.41608000	0.64337300
H	-1.36515500	2.07948300	0.18768200
H	-0.59174200	3.37541500	0.65417000
H	-2.79294800	0.45554100	-0.27809500
O	-2.70417300	1.39516000	-0.53689100
H	-2.71704500	1.39955500	-1.49810500
B1b3			
S	1.49946100	0.06583300	0.07221600
O	0.87129900	0.80734600	-0.98011900
O	2.35697600	0.70012200	1.01330100
O	2.30489800	-1.07531700	-0.68991200
H	2.94390800	-1.47827400	-0.08481000
O	0.43390300	-0.72021100	0.88674500
H	-0.29879000	-1.13834600	0.32213400
O	-2.69321300	-1.54636100	-0.32583700
H	-2.67176900	-0.65576300	0.18025200
O	-1.45240200	-1.97293200	-0.40811800
O	-1.39276900	2.43913200	-0.69791800
H	-1.21842100	3.37536200	-0.57461800
H	-0.53868300	2.01560600	-0.89064500
H	-2.21800400	0.71590000	1.77775300
O	-2.64870700	0.70455700	0.91824500
H	-2.22950300	1.42150100	0.38339300
B1n1			
S	-0.71478600	-0.01727900	0.48235000
O	0.47662600	-0.69843600	0.92146900
O	-1.90714400	-0.12248600	1.26358300
O	-0.99381500	-0.53290300	-0.96814300
H	-1.97079100	-0.45693500	-1.16804400
O	-0.40556200	1.48865100	0.30923900
H	0.55474400	1.65897600	0.00496900
O	2.79295100	-1.57270600	-0.06800300
H	1.90552400	-1.27839200	0.27849900
O	3.37434300	-0.49835200	-0.56016200
O	2.00906200	1.90673500	-0.45946300
H	2.51749800	1.06548200	-0.48670400
H	2.51948200	2.51903900	0.07812800
O	-3.63358400	-0.38487100	-1.05061000
H	-4.12958300	0.34306400	-1.43666400
H	-3.66331500	-0.25982100	-0.09106300

B1n2

S	-1.53922600	-0.39852800	-0.16835100
O	-0.82148900	0.61196500	-0.90516700
O	-2.60502500	-1.10541200	-0.78920200
O	-2.11268700	0.40066800	1.09208700
H	-2.78992200	-0.13351100	1.53013800
O	-0.55883600	-1.40225900	0.44262500
H	0.39762300	-0.99391100	0.65869200
O	0.74634800	2.71998700	-0.45224200
H	0.12276700	1.95690100	-0.60400800
O	1.74856600	2.24156800	0.25697300
O	1.68702700	-0.46871500	0.95018500
H	1.73463800	0.48008700	0.71027100
H	2.40930800	-0.92235600	0.47518100
H	4.63923600	-1.69640000	-0.16260500
O	3.71729300	-1.80629300	-0.41281200
H	3.70439500	-1.84642900	-1.37363700

B1n3

S	1.66675400	-0.57130800	-0.11569500
O	0.34669200	-0.61342400	-0.68951300
O	2.68960800	-1.42696800	-0.59937400
O	1.41450500	-0.86819400	1.42927800
H	2.25040300	-1.10104100	1.85831500
O	2.19365500	0.87839000	-0.13280800
H	1.44605400	1.57273500	-0.04210400
O	-2.16647800	0.00478600	-0.13818000
H	-1.22298900	-0.26965100	-0.32020700
O	-2.14615000	1.29779000	0.11097200
O	0.31866800	2.60511400	0.10264300
H	-0.56461300	2.17924700	0.08014600
H	0.30471200	3.31174400	-0.54951500
H	-4.16683400	-0.85420900	-0.04167200
O	-5.03542000	-1.26872900	-0.00732700
H	-5.63542900	-0.56801900	0.26062500

B2n1

S	-0.77193700	-0.52455500	0.07803900
O	0.17070300	-1.45788900	-0.47195800
O	-1.89188200	-1.00512400	0.82532200
O	-1.27014400	0.34577200	-1.11960200
H	-2.16590000	0.73213500	-0.89776000
O	-0.02956800	0.48464400	1.00786300
H	0.81189100	0.86099800	0.61091200
O	3.30117100	1.21111300	-0.14515000
H	3.16422800	0.20343600	-0.14337200

O	2.14577600	1.75182500	0.17514900
O	2.88322800	-1.34694300	-0.20773900
H	3.17831300	-1.90896200	0.51394400
H	1.92682700	-1.51770000	-0.32490200
H	-3.63404100	0.32614900	0.42766800
O	-3.68788600	1.00017900	-0.26515800
H	-3.90151800	1.82819400	0.17507300
B2n2			
S	-1.33665800	-0.34825700	0.02850000
O	-0.94392700	-1.67735000	-0.36568100
O	-2.70265600	-0.08385000	0.30096900
O	-0.75852500	0.58785400	-1.08739000
H	-0.56802700	1.51679900	-0.77927100
O	-0.52587100	0.09201200	1.30482400
H	0.44412000	0.14796100	1.11570400
O	2.85964700	0.06425800	-0.09317500
H	2.45014400	-0.87186500	-0.17767100
O	2.02284500	0.75879700	0.64533500
O	1.71892200	-2.22170800	-0.36085000
H	1.88909600	-2.94442400	0.24948800
H	0.74200300	-2.12793100	-0.42447700
H	1.09638100	2.66273600	-0.00785600
O	0.20713200	2.92149700	-0.28593400
H	0.31227500	3.65676000	-0.89669800
B2n3			
S	1.55669000	-0.47160400	0.00760400
O	0.66293200	-0.73896300	1.09502500
O	2.29725300	-1.51540100	-0.61106200
O	2.56774800	0.61150200	0.59467500
H	3.34098700	0.67532100	0.01616400
O	0.81687300	0.29685200	-1.12254300
H	0.19938000	1.02929800	-0.79519300
O	-1.85771000	2.28625100	0.08043500
H	-1.95532500	1.32006200	0.43340300
O	-0.71858200	2.34125200	-0.57351900
O	-2.04749700	-0.08228000	0.98704500
H	-2.56210400	-0.74040300	0.48602400
H	-1.16100100	-0.45573000	1.13148800
H	-3.55713500	-2.02798700	-1.39019900
O	-3.56525000	-1.95833700	-0.43131500
H	-4.45799400	-2.18190600	-0.15327800