

Supplementary Information

Does H_4SO_5 exist?

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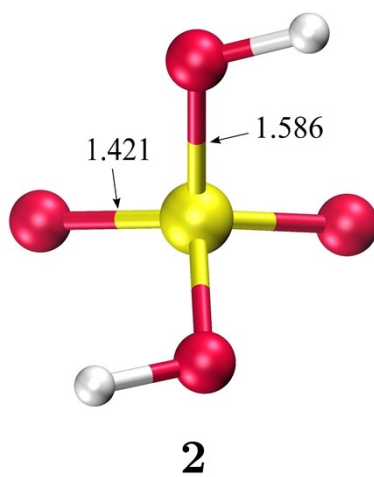


Figure 1-SI. MP2/def2-TZVP structure of H₂SO₄ (**2**). Bond lengths in Å.

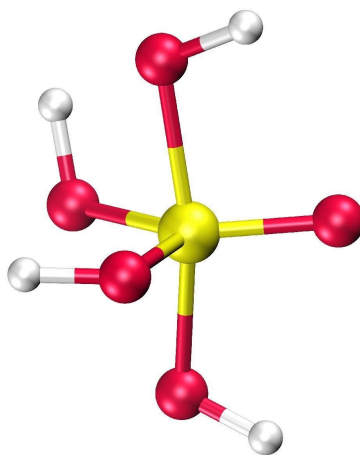


Figure 2-SI. Transition state for the transformation of the *trans* form into *cis* one of **1**.

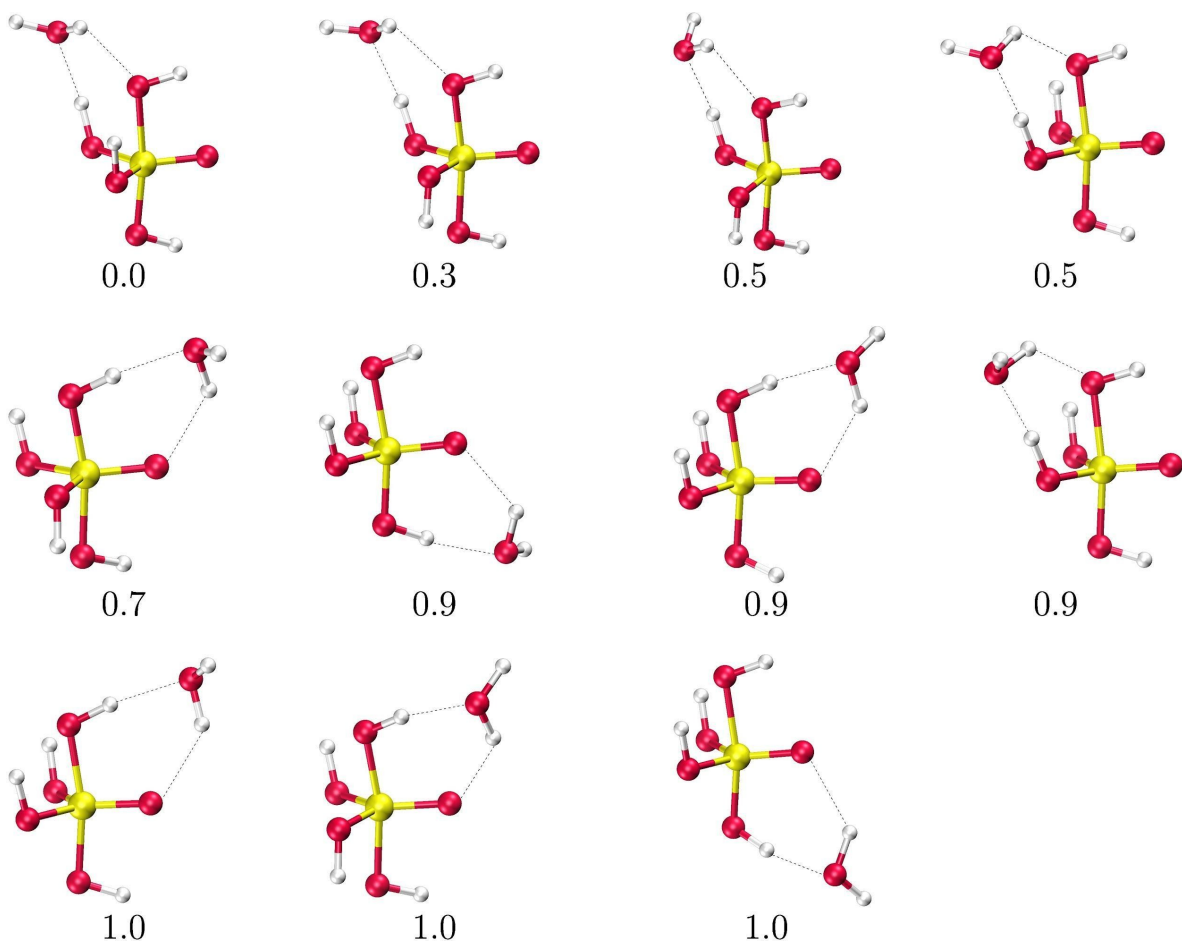


Figure 3-SI. MP2/def2-TZVP structures of the lowest energy isomers of $\text{H}_4\text{SO}_5 \cdot x\text{H}_2\text{O}$ complex. Relative energies and bond lengths in kcal/mol and Å, respectively.

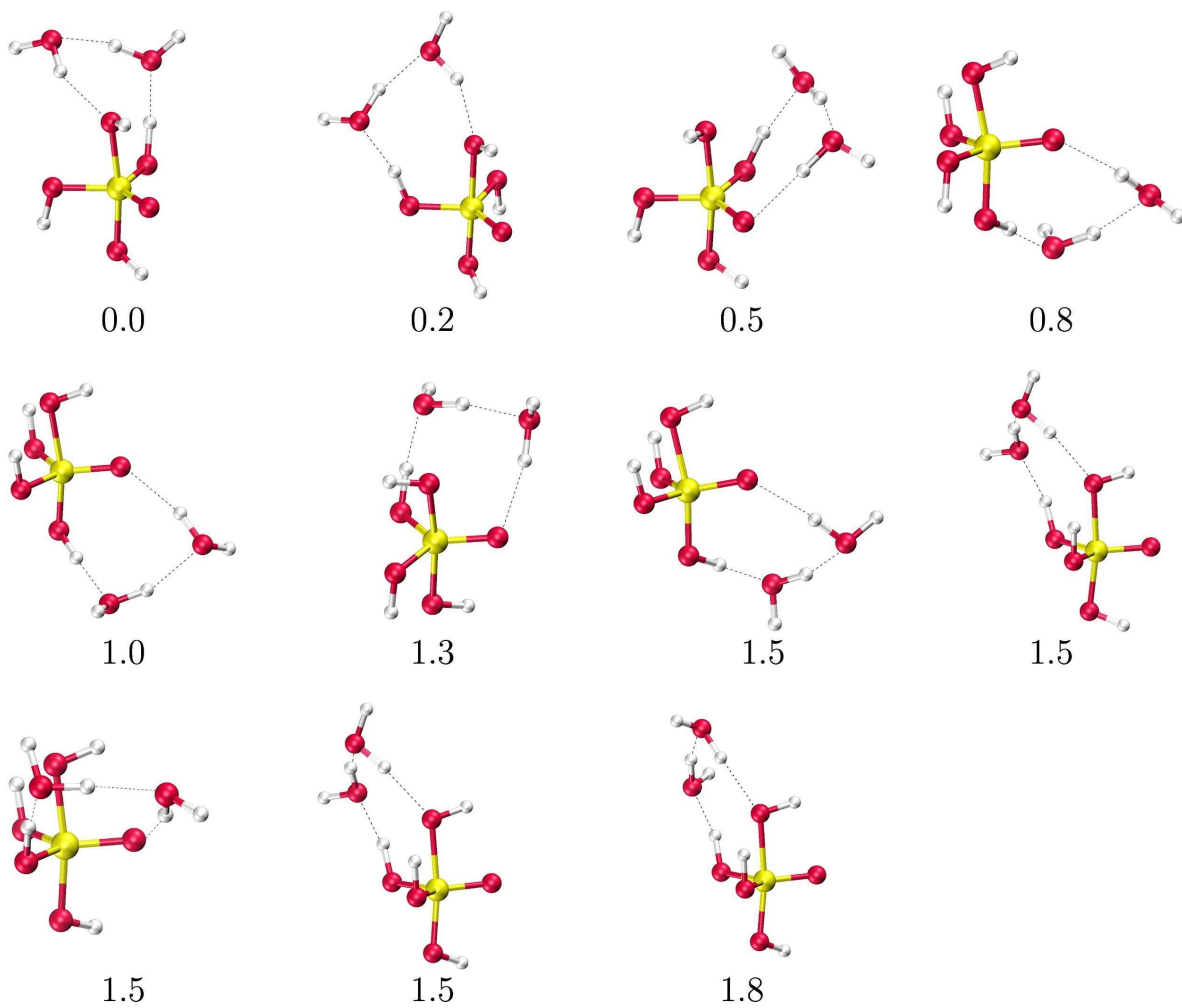


Figure 4-SI. MP2/def2-TZVP structures of the lowest energy isomers of $\text{H}_4\text{SO}_5 \times \times \times 2\text{H}_2\text{O}$ complex. Relative energies and bond lengths in kcal/mol and Å, respectively.

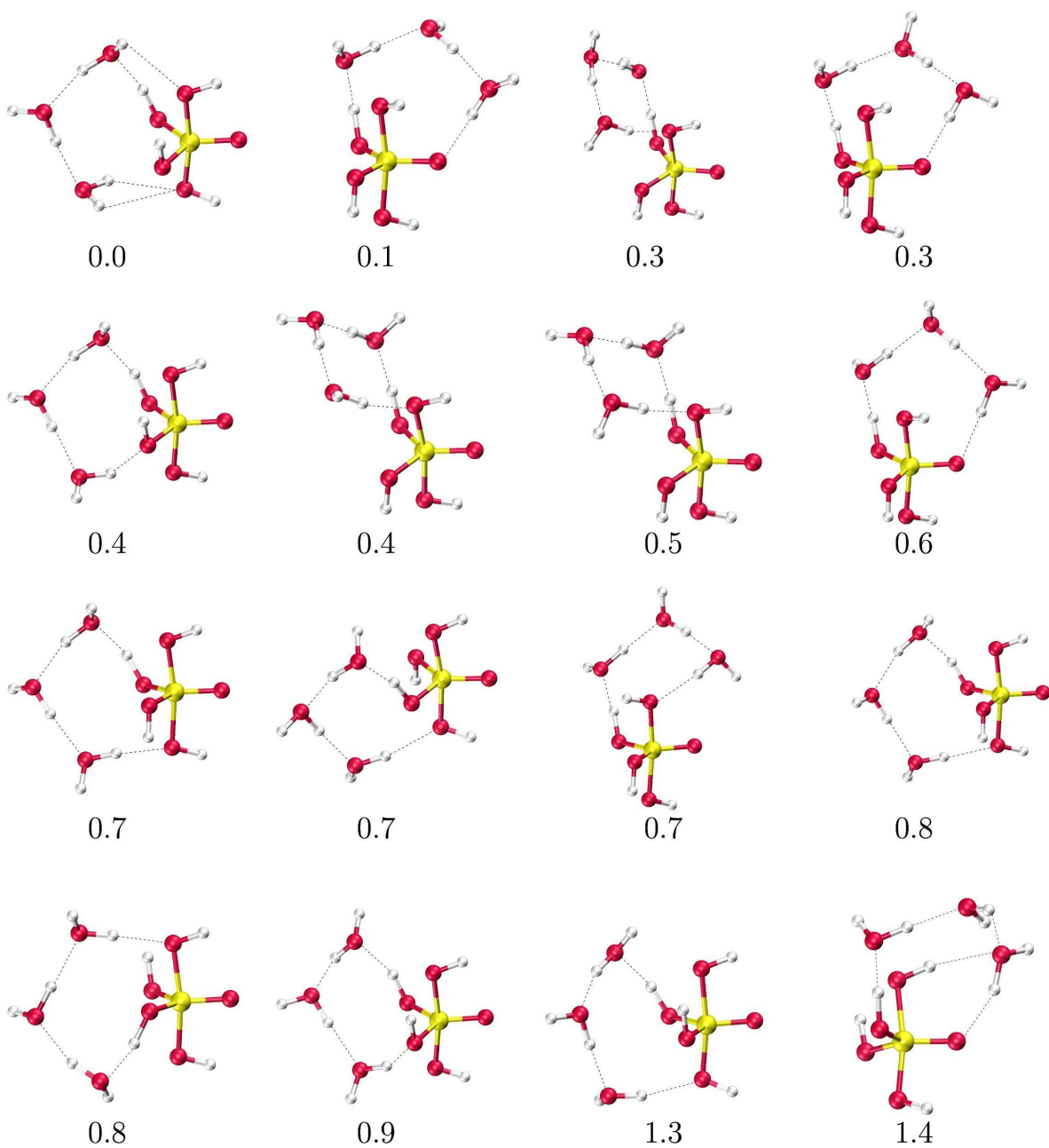


Figure 5-SI. MP2/def2-TZVP structures of the lowest energy isomers of $\text{H}_4\text{SO}_5 \times \times \times 3\text{H}_2\text{O}$ complex. Relative energies and bond lengths in kcal/mol and Å, respectively.

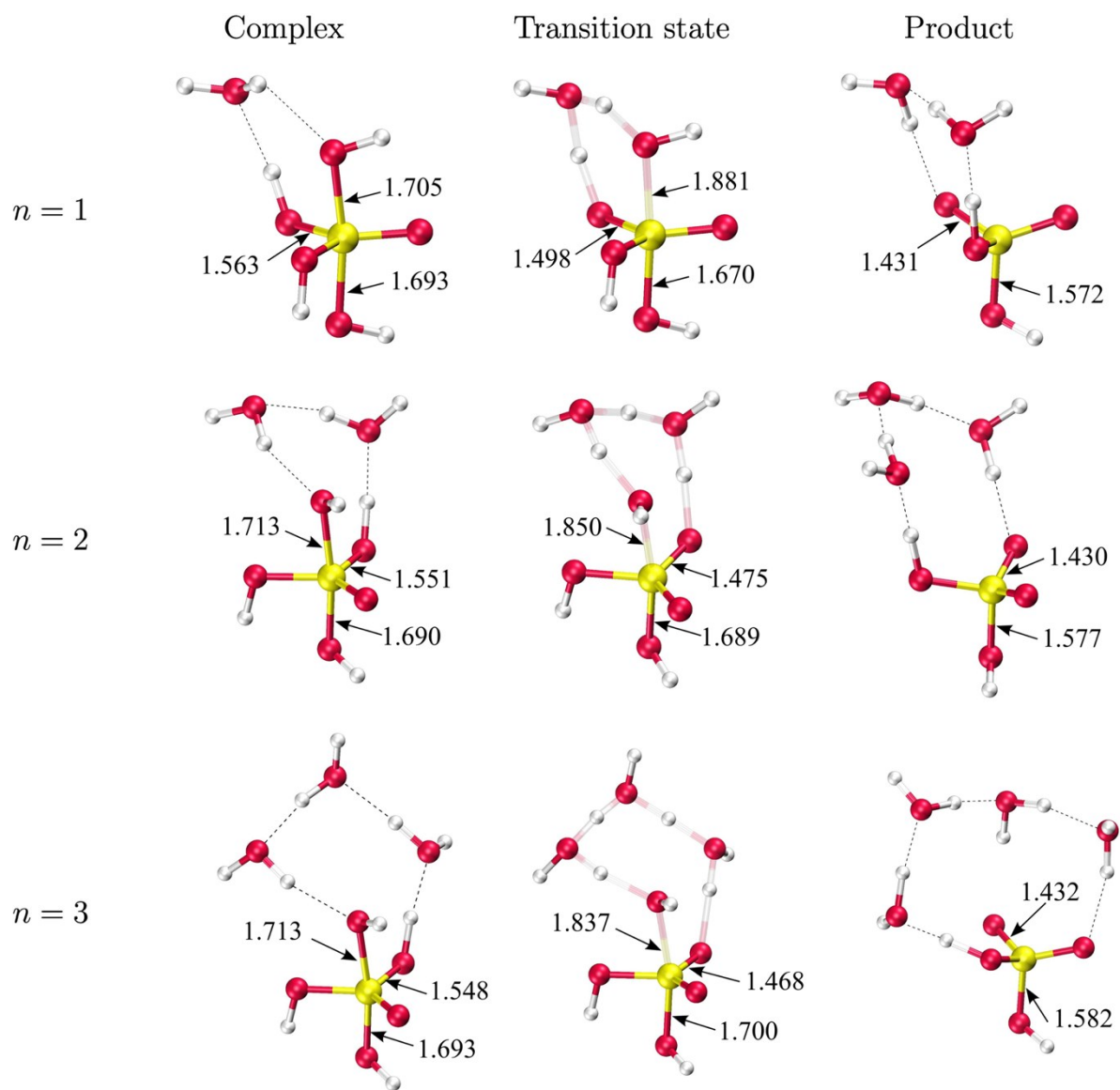


Figure 6-SI. MP2/def2-TZVP structures of the $\text{H}_4\text{SO}_5(\text{H}_2\text{O})_n$ ($n = 1-3$) clusters and the transition states related to the dehydration of **1B**.

Cartesian coordinates for the structures of the Figure 1-SI

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H2SO4 (2)

S	0.000000000	0.000000000	0.158357000
O	0.000000000	1.256503000	0.822138000
O	-1.232058000	0.049530000	-0.839581000
O	1.232058000	-0.049530000	-0.839581000
O	0.000000000	-1.256503000	0.822138000
H	-1.423905000	-0.859019000	-1.127315000
H	1.423905000	0.859019000	-1.127315000

Cartesian coordinates for the structures of the Figure 2-SI

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H4SO5_TS

O	0.0843170	-1.4923470	0.3707000
H	1.0363050	-1.6507250	0.4775380
H	-2.0861980	0.6037050	0.2310660
O	-0.0654440	0.4168570	-1.4838130
S	-0.0400890	0.0717290	0.0832290
O	-0.0820240	1.2521280	0.9115580
O	1.6780240	-0.0000410	0.0503180
O	-1.6576370	-0.2505780	0.1123900
H	0.0485230	-0.3951990	-1.9932140
H	1.9849090	0.8864020	0.2637260

Cartesian coordinates for the structures of the Figure 2

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H4SO5 (1A)

O	-0.1302560	-1.4225030	0.3522900
H	-1.1457320	-1.3263250	0.2785920
H	2.2581430	0.2911850	-0.4140710
O	-0.0927930	1.0777610	1.0036220
S	0.2163150	0.0153680	-0.0838580
O	0.2188090	0.3992500	-1.4573520
O	-1.8973260	0.0093140	-0.0103560
O	1.7500850	-0.1282570	0.2910070
H	-1.0947470	1.0948100	0.9170060
H	-2.2668670	0.2099210	-0.8734780

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H4SO5 (1B)

O	-0.088792000	0.784469000	1.319128000
H	-1.043825000	0.909177000	1.470393000
H	1.992411000	-0.822013000	0.347177000
O	0.088665000	0.801188000	-1.309180000
S	0.000019000	-0.097489000	-0.000671000
O	0.000091000	-1.549367000	-0.009893000
O	-1.674854000	0.067773000	-0.130759000
O	1.674865000	0.066236000	0.131891000
H	1.043674000	0.927909000	-1.458896000
H	-1.992357000	-0.817649000	-0.357446000

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TSA

O	-0.1302560	-1.4225030	0.3522900
H	-1.1457320	-1.3263250	0.2785920
H	2.2581430	0.2911850	-0.4140710
O	-0.0927930	1.0777610	1.0036220
S	0.2163150	0.0153680	-0.0838580
O	0.2188090	0.3992500	-1.4573520
O	-1.8973260	0.0093140	-0.0103560
O	1.7500850	-0.1282570	0.2910070
H	-1.0947470	1.0948100	0.9170060
H	-2.2668670	0.2099210	-0.8734780

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TSB

O	-0.2870130	-0.4603170	1.3779940
H	-1.3936320	-0.3035730	1.0386340
H	2.1026200	-0.8111730	-0.1848020
O	0.1019070	1.4782550	-0.3117990
S	0.1142520	-0.0803490	-0.0443090
O	0.0892440	-0.9947540	-1.1558470
O	-1.8096860	0.1657160	-0.0808720
O	1.7263340	-0.0449470	0.2735170
H	1.0353840	1.7542180	-0.2709060
H	-2.1386950	-0.5055080	-0.6979390

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2A-H₂O

O	0.9167830	1.2827280	-0.6388250
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S	0.5849660	-0.0672850	0.1302120
O	-0.1933970	0.3451840	1.2573030
O	-0.3320110	-0.8258760	-0.8754880
O	1.7859140	-0.8185990	0.2609630
H	1.6302530	1.0987740	-1.2723450
H	-1.2805460	-0.5305750	-0.7222380
O	-2.6732280	0.0890490	-0.1181800
H	-3.4241270	-0.4752070	0.0975530
H	-2.3175210	0.4036870	0.7274660

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2B-H₂O

O	-1.5790050	-1.0719580	0.3277480
H	3.4380250	-0.5394780	0.0619150
H	-0.7566860	1.9036470	-0.5574230
O	0.3599160	-0.5551110	-1.0405340
S	-0.5855510	-0.0868980	0.1088480
O	0.2315610	0.4251090	1.1780250
O	2.7136260	0.0823490	-0.0699680
O	-1.3477130	1.1331330	-0.5545540
H	1.3093540	-0.3580810	-0.7800570
H	2.3510550	0.2760980	0.8082610

Cartesian coordinates for the structures of the Figure 3

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H₄SO₅-H₂O Complex n=1

S	0.5841340	0.0232020	-0.0747410
O	-0.4265630	-1.1542240	-0.0092160
O	-0.8407950	1.1785570	-0.0391790
O	0.9009060	0.6394750	1.3496980
H	-1.3881670	-0.8792720	-0.0687470
O	1.0425420	0.5931930	-1.3217050
H	0.2262950	1.3291300	1.4656660
O	1.8071750	-1.0143050	0.1757210
H	-0.6849130	1.7260190	-0.8151470
H	-2.5769770	0.4701160	0.0031530
H	2.3378380	-0.9852860	-0.6267030
O	-2.9553370	-0.4227860	-0.0876270
H	-3.4836420	-0.5912290	0.6960930

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H4SO5-H2O_TS Transition state n=1

S	0.6037510	-0.0063130	-0.0765220
O	-0.3671590	-1.1611630	0.1770700
O	-1.0195610	1.2257860	-0.0533450
O	0.8886190	0.8593170	1.1932080
H	-1.3840140	-0.9607330	0.0709050
O	0.8753790	0.4333780	-1.4140360
H	0.1154730	1.4764210	1.1676260
O	1.9060420	-0.8835030	0.2496430
H	-0.9106040	1.7344880	-0.8618040
H	-2.3864890	0.3607160	-0.0567290
H	2.2518060	-1.1882430	-0.5970850
O	-2.7869670	-0.5576630	-0.0571170
H	-3.3170130	-0.6508540	0.7380560

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H2SO4-2H2O Product n=1

O	0.1567650	1.3089200	-0.0765580
H	-1.6939820	1.4363520	0.0604310
H	2.8963650	-0.3309930	-0.2994130
O	0.2991140	-1.0145070	-0.8076350
S	0.8835900	0.0877000	0.0926520
O	1.1118890	-0.4071040	1.4098320
O	-2.0766320	-1.4326840	-0.0969150
O	2.2637630	0.3248590	-0.6223260
H	-0.6681470	-1.2475300	-0.5067340
H	-2.1887680	-1.8443590	0.7637790
O	-2.6251710	1.1525850	0.0853440
H	-3.0753850	1.6417600	-0.6065000
H	-2.4453440	-0.5149830	-0.0279430

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H4SO5-2H2O Complex n=2

S	1.0175370	-0.0385950	0.0731810
O	-0.5618060	-0.8821780	0.5372570
O	0.1931270	1.2245110	-0.2286870
O	1.0251270	-1.0888150	-1.1165110
H	-0.7976430	1.1927590	0.0091380
H	0.2770190	-1.6780340	-0.9268000
H	-0.4056110	-1.1241620	1.4548350
O	1.5778680	-0.3555340	1.3667340
O	2.3127590	0.6821250	-0.5876990

H	-2.2144640	-1.1151440	-0.0241920
H	-2.8158370	0.7211220	-0.0110000
O	-3.1280110	-0.9389390	-0.3345510
O	-2.3021520	1.5380070	0.1843410
H	3.0617890	0.4246440	-0.0403670
H	-2.6067830	2.2145670	-0.4247660
H	-3.7143670	-1.4516440	0.2251690

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H4SO5-2H2O_TS Transition state n=2

S	1.0540420	-0.0197510	0.0645370
O	-0.7003680	-1.0235590	0.4004120
O	0.1995490	1.1845780	-0.2525470
H	-0.8394110	1.1977880	0.0004910
O	1.0890680	-1.1026440	-1.0702650
H	-0.5750280	-1.3498960	1.2951210
H	0.2878620	-1.6332520	-0.8337070
O	1.4556160	-0.3733050	1.3949060
O	2.3695190	0.7082240	-0.4986820
H	-2.2641420	-1.0560530	-0.0708850
O	-2.1769790	1.5318040	0.2094170
H	-2.7323220	0.7226290	0.0175470
H	3.1208290	0.3186260	-0.0367380
O	-3.1861430	-0.7833760	-0.3403510
H	-2.4676530	2.2301060	-0.3825460
H	-3.7969140	-1.2477000	0.2350170

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H2SO4-3H2O Product n=2

S	-1.1242140	-0.0750060	-0.0316480
O	1.5711680	-2.1121120	0.1979910
O	-0.8386070	1.3497820	-0.4955770
H	0.1494530	1.6652810	-0.2232940
O	-0.6027550	-0.2738270	1.2903180
H	0.8410440	-2.0267200	-0.4341240
H	1.1365940	-1.9448310	1.0421490
O	-0.7957600	-1.0358790	-1.0352340
O	-2.6976830	-0.0685750	0.0200480
H	2.5818620	-0.7777820	-0.0570530
O	1.4310920	2.0778960	0.1065820
H	2.0925090	1.3370830	-0.0394750
H	-2.9888230	0.4920890	0.7517000

O	3.0618070	0.0813290	-0.1649200
H	1.4973500	2.3190060	1.0342090
H	3.6433280	-0.0129510	-0.9214020

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H4SO5-3H2O Complex n=3

O	0.0613410	-0.2253260	1.0766040
H	-0.5850320	-1.0287820	0.9038200
S	1.1635800	-0.0290380	0.0161000
O	0.7523240	-1.5936380	-0.6811560
O	-1.6999380	-1.9385420	0.6544430
H	1.5722120	-2.0933240	-0.6217510
H	-1.3330860	-2.4504890	-0.0736640
O	2.5535650	-0.3904400	0.1920940
O	1.3018480	1.5339700	0.5416820
O	0.6021100	0.5746500	-1.3617260
H	-2.3711370	-1.3284160	0.2572840
H	0.3984250	-0.2049970	-1.9028220
H	2.2448000	1.7248780	0.5462530
H	-1.0753820	1.9160320	0.8782210
H	-2.6690410	0.8100630	-0.2430200
O	-3.1764070	-0.0135480	-0.4299740
O	-1.6136350	2.1442910	0.1104980
H	-4.0941330	0.1806390	-0.2315510
H	-0.9545650	2.2076640	-0.5900970

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H4SO5-3H2O_TS Transition state n=3

O	-0.0946670	-0.1576310	-1.1161740
S	-1.1415110	-0.0020600	-0.0500650
H	0.7509990	-1.0244100	-0.9827460
O	-0.5826670	0.5553590	1.3490810
O	-0.5839070	-1.6470490	0.7024880
H	-0.3700070	-0.2625590	1.8363340
O	-1.4009540	1.5559260	-0.5113770
H	1.0834740	1.9102920	-0.8256550
H	0.9698810	2.1215520	0.6587250
O	-2.4959460	-0.4862760	-0.1391950
H	-1.3815720	-2.1824110	0.6793270
O	1.5694300	-1.8206580	-0.6808820
O	1.6242150	2.1055290	-0.0500070
H	2.2909100	-1.2614130	-0.2615770

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H	1.0048730	-2.1775180	0.0434580
H	-2.3097160	1.7657490	-0.2710330
H	2.6677470	0.7801940	0.2390280
O	3.1504020	-0.0703180	0.3861590
H	4.0703380	0.0844450	0.1644430

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H2SO4-4H2O Product n=3

O	-0.4546340	-0.1322530	1.2083300
S	-1.2870530	-0.1530080	0.0057750
H	0.7992020	0.6707050	1.2040020
O	-0.9869750	-1.2540880	-0.8874670
O	0.7139900	2.7886220	-0.6671190
H	1.0898890	2.8696670	-1.5466870
O	-2.7238430	-0.4404860	0.6197940
H	1.1867470	-3.0103910	0.3547030
H	0.5126720	-2.0966940	-0.6808710
O	-1.3697970	1.1301850	-0.6670960
H	-0.1329510	2.2908150	-0.7674930
O	1.6746560	1.1908560	1.0430890
O	1.3758950	-2.5010200	-0.4370240
H	2.3183580	0.5162370	0.6008630
H	1.4180730	1.9035700	0.3514120
H	-3.3450580	-0.5497050	-0.1117990
H	2.4775310	-1.3306730	-0.2654100
O	3.0642610	-0.5292720	-0.1373620
H	3.9199660	-0.8357490	0.1677140

Cartesian coordinates for the structures of the Figure 6-SI

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H4SO5-H2O Complex n=1

S	0.538149000	0.091999000	-0.071989000
O	-0.460441000	-1.079386000	-0.345650000
O	-0.777086000	1.152493000	0.160747000
H	-1.410760000	-0.772110000	-0.319931000
O	0.806909000	0.289012000	1.488680000
O	1.145607000	0.902892000	-1.114787000
O	1.769886000	-1.069514000	-0.047414000
H	-0.521455000	1.935791000	-0.346532000
H	1.574461000	-0.283259000	1.673452000
H	2.308133000	-0.866221000	-0.825005000

H	-2.734113000	0.504201000	0.243612000
O	-3.018973000	-0.347794000	-0.120698000
H	-3.553869000	-0.772007000	0.559193000

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H4SO5-H2O_TS Transition state n=1

O	-0.409990000	-1.143304000	-0.245315000
H	-1.626510000	-0.952446000	-0.187846000
H	2.376183000	-0.716530000	-0.794812000
O	0.734468000	0.439086000	1.439394000
S	0.501312000	0.037574000	-0.087667000
O	0.944798000	0.870683000	-1.187253000
O	-0.981524000	1.165964000	0.152857000
O	1.876348000	-0.920405000	0.008422000
H	1.560222000	-0.021366000	1.677655000
H	-0.828844000	1.842410000	-0.522323000
O	-2.693941000	-0.471812000	-0.108858000
H	-3.126121000	-0.725136000	0.716995000
H	-2.137187000	0.450194000	0.039021000

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H2SO4-2H2O Product n=1

S	-0.992754000	-0.089762000	-0.126918000
O	-0.081614000	-0.979213000	-0.785851000
O	-0.464183000	1.357617000	-0.171736000
H	0.560427000	1.389067000	-0.059631000
H	1.718617000	-1.396912000	-0.361224000
O	-0.846340000	-0.480490000	1.412869000
O	-2.373621000	-0.059425000	-0.465742000
H	2.417833000	0.510789000	0.113187000
O	2.625603000	-1.169121000	-0.089183000
O	2.058081000	1.431680000	0.139680000
H	-1.560863000	-0.039642000	1.902202000
H	2.847687000	-1.773111000	0.626896000
H	2.556945000	1.937629000	-0.511041000

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H4SO5-2H2O Complex n=2

S	0.924876000	-0.011404000	0.119835000
O	-0.473520000	-0.489551000	0.985901000
O	0.150629000	1.195137000	-0.471682000
H	-0.820936000	1.257587000	-0.176693000

O	0.674956000	-1.346401000	-0.730859000
H	-0.142231000	-0.653445000	1.880063000
O	1.755304000	0.058025000	1.311568000
H	-1.976421000	-1.252788000	0.200537000
H	1.379477000	-1.334862000	-1.405008000
O	2.178606000	0.334069000	-0.959987000
H	-2.758604000	0.604357000	-0.221293000
O	-2.381494000	1.510153000	-0.150285000
H	2.918307000	0.597912000	-0.395118000
O	-2.872860000	-1.159744000	-0.173649000
H	-2.749172000	1.884445000	0.657444000
H	-2.901415000	-1.734260000	-0.945338000

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H4SO5-2H2O_TS Transition state n=2

S	-0.890225000	0.029143000	-0.118130000
O	0.524204000	-0.807571000	-0.966441000
O	-0.119493000	1.286938000	-0.085046000
H	1.287082000	1.359633000	-0.110070000
O	-0.476432000	-0.985563000	1.079668000
H	0.093415000	-1.437301000	-1.560218000
O	-1.781033000	-0.400523000	-1.180427000
H	1.682669000	-1.144788000	-0.168822000
H	-1.138807000	-0.787541000	1.767550000
O	-2.113300000	0.607055000	0.910522000
H	2.568377000	0.247895000	0.226226000
O	2.342282000	1.357520000	-0.013604000
H	-2.921020000	0.523638000	0.384473000
O	2.569651000	-1.001942000	0.372891000
H	2.716216000	1.593910000	-0.872746000
H	2.388644000	-1.269043000	1.283166000

16

H2SO4-3H2O Product n=2

S	-1.042531000	-0.029220000	-0.026759000
O	-0.446097000	-0.075871000	1.326556000
O	-0.656136000	-1.152610000	-0.854254000
O	-0.886968000	1.282609000	-0.638455000
H	1.010063000	0.014504000	1.297585000
H	0.964154000	-1.815468000	-0.768336000
H	0.741238000	1.956929000	-0.631830000
O	2.029946000	0.057557000	1.057022000

H	2.082725000	0.875840000	0.451095000
H	2.150275000	-0.765736000	0.468425000
O	-2.600319000	-0.249510000	0.192592000
O	1.702967000	2.086464000	-0.455580000
O	1.920387000	-1.918956000	-0.550826000
H	-2.951425000	0.547119000	0.622467000
H	2.118421000	2.261389000	-1.306599000
H	2.054805000	-2.844506000	-0.321092000

19

H4SO5-3H2O Complex n=3

S	-1.017790000	-0.079819000	0.004084000
O	0.355104000	-0.640504000	-0.959037000
O	-0.233087000	-0.298238000	1.242426000
H	1.119993000	0.086625000	1.221660000
O	-1.048713000	1.217880000	-0.696028000
H	0.112355000	-0.490201000	-1.884368000
H	0.584506000	1.920491000	-0.772887000
O	-1.756598000	-1.360655000	-0.622561000
H	2.046726000	1.164468000	0.454245000
H	1.766066000	-1.592725000	-0.608249000
O	2.132201000	0.400653000	1.117306000
O	-2.484568000	0.190847000	0.841733000
H	2.549021000	-0.387983000	0.640193000
O	1.510805000	2.212737000	-0.598792000
H	-2.627153000	1.144743000	0.780638000
H	-2.667162000	-1.290054000	-0.279324000
O	2.677960000	-1.704229000	-0.247767000
H	1.461026000	3.151959000	-0.390951000
H	2.714428000	-2.578155000	0.155450000

19

H4SO5-3H2O_TS Transition state n=3

S	-1.029649000	-0.022415000	0.036226000
O	0.066877000	-1.075174000	-1.019356000
O	-0.232974000	-0.391588000	1.200881000
H	1.371131000	0.158304000	1.424559000
O	-0.761775000	1.137535000	-0.831584000
H	-0.054022000	-0.783661000	-1.933708000
H	0.896005000	1.763479000	-0.885979000
O	-2.125267000	-1.090054000	-0.437789000

H	2.303520000	1.018414000	0.518614000
H	1.344380000	-1.498445000	-0.612967000
O	2.325702000	0.257306000	1.167461000
O	-2.268332000	0.749085000	0.922109000
H	2.436429000	-0.736563000	0.510708000
O	1.838660000	1.996685000	-0.729403000
H	-2.315541000	1.637582000	0.543412000
H	-2.942214000	-0.769770000	-0.012085000
O	2.315805000	-1.691743000	-0.230297000
H	1.882442000	2.958159000	-0.723736000
H	2.282685000	-2.525270000	0.255399000

19

H4SO5-4H2O Product n=3

S	1.318181000	-0.254368000	0.039266000
O	0.554893000	0.021354000	1.273948000
H	-0.658498000	0.827821000	1.173196000
O	0.862207000	-1.425797000	-0.671556000
O	1.490259000	0.945382000	-0.769033000
H	-0.758085000	-2.080601000	-0.586096000
O	-1.525460000	1.377180000	0.996995000
H	0.281139000	2.162374000	-1.021669000
H	-1.290302000	1.976859000	0.211450000
H	-2.251036000	0.703786000	0.719361000
O	2.770956000	-0.675483000	0.535753000
O	-0.532560000	2.713795000	-0.938928000
O	-1.708209000	-2.329351000	-0.629176000
H	-2.705233000	-1.137464000	-0.109711000
H	3.179438000	0.105502000	0.942234000
O	-3.207390000	-0.358326000	0.258031000
H	-0.884041000	2.824001000	-1.828410000
H	-1.820744000	-2.750241000	-1.487430000
H	-3.821093000	-0.712190000	0.910541000

Cartesian coordinates for the structures of the Figure 4

17

H4SO5-H2SO4 Complex

H	0.267317000	-0.077423000	1.448596000
O	0.738086000	1.385067000	-0.164914000
H	-0.747079000	-1.035719000	-1.081473000

O	0.990047000	-0.659316000	-1.148586000
S	1.719182000	-0.021732000	-0.065003000
H	-0.912411000	1.449839000	-0.530276000
O	-1.370418000	-0.139290000	1.277795000
O	1.245540000	-0.303618000	1.398226000
S	-2.205463000	-0.063941000	0.095903000
O	-1.717292000	-1.145184000	-0.925645000
O	-1.889543000	1.284370000	-0.623874000
H	1.140984000	2.091742000	0.363566000
O	2.924259000	1.014825000	-0.170242000
O	2.910135000	-1.177730000	0.084247000
H	2.498944000	-2.037786000	-0.086012000
O	-3.607254000	-0.197423000	0.213954000
H	3.744266000	0.486496000	-0.136498000

17

H4SO5-H2SO4_TS Transition state			
H	-0.072304000	-0.179816000	1.301468000
O	0.687832000	1.505754000	-0.243346000
H	-0.786739000	-1.095293000	-1.163977000
O	1.000680000	-0.585801000	-1.210261000
S	1.676788000	-0.061737000	-0.041249000
H	-0.537193000	1.377449000	-0.470452000
O	-1.338717000	-0.159907000	1.311259000
O	1.067228000	-0.288826000	1.323136000
S	-2.130888000	-0.033563000	0.061241000
O	-1.713605000	-1.234155000	-0.862909000
O	-1.659826000	1.195987000	-0.667453000
H	0.889764000	2.128334000	0.472516000
O	2.852317000	0.998902000	-0.051192000
O	2.842364000	-1.220828000	0.119247000
H	2.438542000	-2.074000000	-0.099069000
O	-3.531440000	-0.100688000	0.233688000
H	3.678863000	0.484619000	0.022276000

17

H4SO5-H2SO4 Product			
H	-0.616049000	-0.480793000	1.429616000
O	0.637550000	2.714645000	-0.123677000
H	-0.640190000	-1.137793000	-1.138799000
O	1.100359000	-0.963292000	-1.089412000

S	1.794135000	-0.361209000	0.018306000
H	-0.219800000	2.230624000	-0.197490000
O	-1.598543000	-0.564944000	1.376239000
O	1.099095000	-0.301167000	1.271811000
S	-2.111958000	-0.109062000	-0.021638000
O	-1.613278000	-1.217150000	-0.992792000
O	-1.441557000	1.118009000	-0.371906000
H	0.634077000	3.173740000	0.721007000
O	2.349839000	0.993602000	-0.356915000
O	3.094160000	-1.188229000	0.286164000
H	3.453924000	-1.510466000	-0.552379000
O	-3.519377000	-0.158455000	0.004864000
H	1.607215000	1.784862000	-0.243654000