Electronic Supplementary Information

Cyclic Cooperativity Contributions Determine the Hydrogen Bond Strengths in Molecular Clusters

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Table S1 Molecular energies (in a.u.) of various species of **HB1** energy evaluation in cyclic ammonia tetramer **e** by the MTA-based method (*cf.* Scheme 1 in Main text) calculated at the MP2/aug-cc-pVTZ level. See main text for details.

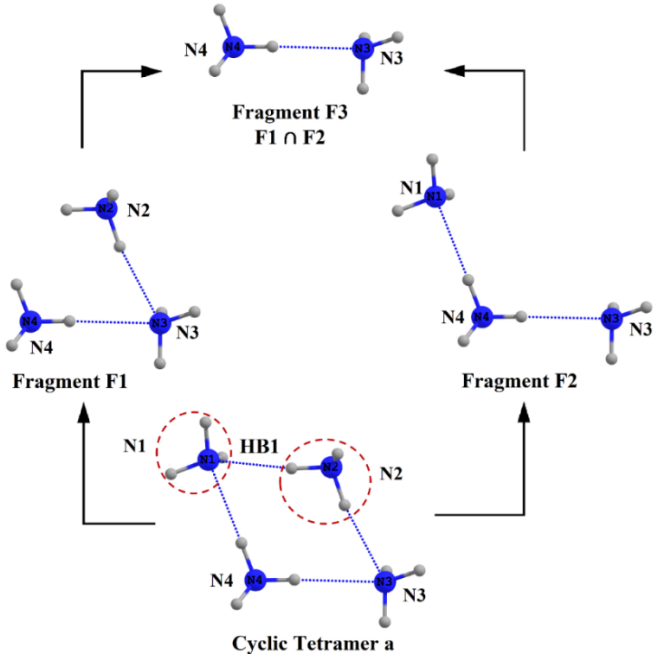
Species	Energy
Ammonia Tetramer (E_M)	-225.9369404
Fragment F1 (E_{F1})	-169.4452682
Fragment F2 (E_{F2})	-169.4444387
Fragment F3 (E_{F3})	-112.9599266
Ammonia dimer ($E_{N2\ldots N1}^{dimer}$)	-112.9599268
Ammonia monomer ($E_{N1}^{monomer}$)	-56.4772137
Ammonia monomer ($E_{N2}^{monomer}$)	-56.4773467

Table S2 Molecular energies (in a.u.) of various species of **HB1** energy evaluation in cyclic ammonia tetramer **a** by the MTA-based method (*cf.* Scheme S1) calculated at the MP2(full)/aug-cc-pVTZ level.

Species	Energy
Ammonia Tetramer **a** (E_a)	-225.9278084
Fragment F1 (E_{F1})	-169.4415391
Fragment F2 (E_{F2})	-169.4412429
Fragment F3 (E_{F3})	-112.9599266

Table S3 Molecular energies (in a.u.) of various species of **HB1** energy evaluation in Parent $(NH_3)_8$ cluster by the MTA-based method (*cf.* Scheme S2) calculated at the MP2(full)/aug-cc-pVTZ level.

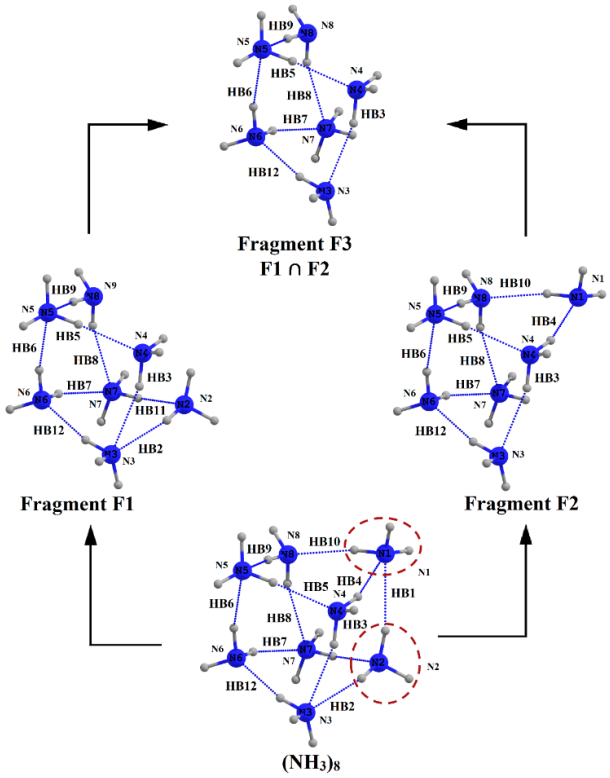
Species	Energy
Parent Cluster	-451.8966258
Fragment F1 (E_{F1})	-395.3993951
Fragment F2 (E_{F2})	-395.3982156
Fragment F3 (E_{F3})	-338.9073695



Scheme S1 MTA based fragmentation scheme for the estimation of strength of HB1 in cyclic tetramer **a** present in **$(NH_3)_8$**.

Scheme S1 presents the MTA-based fragmentation method for the estimation of strength of **HB1** in ammonia tetramer **a** consisting of ammonia molecules N1, N2, N3 and N4. The **HB1** represent the interaction of ammonia molecules N1 and N2. Similar to the fragmentation procedure for tetramer **e** (in main text), the cyclic tetramer **a** is divided into two primary fragments Fragment F1 and Fragment F2, by removing ammonia molecule N1 and N2, respectively. Fragment F3 (consisting of ammonia molecule N3 and N4) is the common overlap fragment of Fragment F1 and F2. Using the single point (SP) energies of these fragments the E_{HB1} in this tetrameric ammonia cycle **a** can be calculated as $E_{HB1}^{cyc\ a}$ = (E_{F1} + E_{F2} – E_{F3}) – E_a = 3.11 kcal/mol at the MP2(full)/aug-cc-pVTZ level. For energies of E_{F1}, E_{F2}, E_{F3} and E_a; see Table S2 in this electronic supplementary information (ESI). However, the calculated $E_{HB1}^{cyc\ a}$ for this cyclic tetramer a includes the cooperativity contribution of ammonia molecule N3 and N4. Recall the discussion in the main text that the interaction energy of **HB1** in an isolated N1…N2 dimer (E_{HB1}^{dimer}= 3.36 kcal/mol) excludes this cooperativity effect. Therefore, the cooperativity contribution (the difference between $E_{HB1}^{cyc\ a}$ and E_{HB1}^{dimer}) to the

HB1 in cyclic tetramer **a** is $E_{coop.}^{cyc\ a} = E_{HB1}^{cyc\ a} - E_{HB1}^{dimer}$ = 3.11 - 3.36 = -0.25 kcal/mol. The negative value of $E_{coop.}^{cyc\ a}$ affirms the anti-cooperativity experienced by HB1 in this cyclic tetramer **a**.



Scheme S2 MTA based fragmentation scheme for the estimation of strength of HB1 in Parent **$(NH_3)_8$** Cluster.

In similar manner, the energy of **HB1** in actual **$(NH_3)_8$** cluster can be calculated (*cf.* Scheme S2) by the MTA-based method by dividing the **$(NH_3)_8$** cluster into two primary fragments, F1 and F2 (obtained by removing ammonia molecules N1 and N2, respectively). A common overlapping fragment of F1 and F2 is fragment F3 consisting of six ammonia molecules (N3, N4, N5, N6, N7 and N8). The energy of **HB** in any molecular cluster can be obtained using the SP energy of these fragments and that of the parent cluster as $E_{HB}^{cluster}$ = (E_{F1} + E_{F2} – E_{F3}) – $E_{cluster}$ …(S1). For the energy of **HB1** in this **$(NH_3)_8$** cluster, this eq. S1 can be written as $E_{HB1}^{(NH_3)_8}$ = (E_{F1} + E_{F2} – E_{F3}) - $E_{(NH3)8}$ = 4.00 kcal/mol at the MP2(full)/aug-cc-pVTZ level. For details of energy of these primary fragments and that of parent **$(NH_3)_8$** cluster, see Table S3 in ESI.

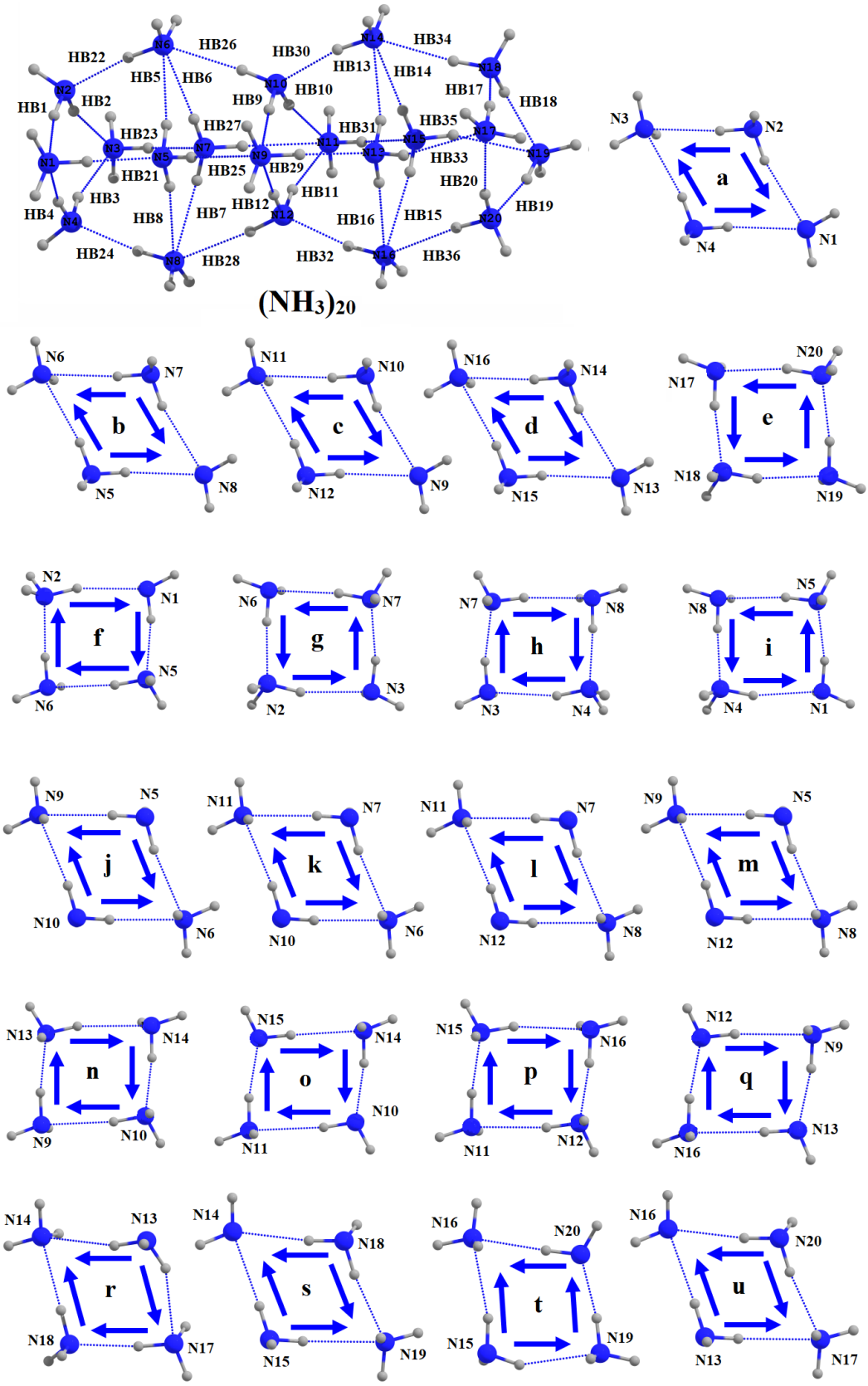


Fig. S1 Structure of $(NH_3)_{20}$ cluster consisting of twenty-one tetrameric cycles denoted by labels **a** to **u**.

Table S4 The hydrogen bond energies (in kcal/mol) in **$(NH_3)_{20}$** cluster obtained by synergetic addition of cyclic cooperativity contributions ($E_{HB}^{Synergetic}$) and that by MTA-based method employing actual cluster ($E_{HB}^{(NH_3)_{20}}$). The hydrogen bond energy in the respective dimer species (E_{HB}^{Dimer}**)** is also provided (kcal/mol). All the calculations were performed at MP2/aug-cc-pVTZ level of theory. See Fig. S1 and main text for details.

HB	E_{HB}^{Dimer}	$E_{coop.}^{Cycle1}$	$E_{coop.}^{Cycle2}$	$E_{coop.}^{Cycle3}$	$E_{HB}^{Synergetic}$	$E_{HB}^{(NH_3)_{20}}$	$\lvert\Delta E_{\mathrm{HB}}\rvert$
HB1	3.04	-0.22 (-a)	1.26 (+f)	-	4.07	3.88	0.19
HB2	3.04	-0.22 (-a)	1.26 (+g)	-	4.08	3.89	0.19
HB3	3.04	-0.22 (-a)	1.26 (+h)	-	4.07	3.88	0.19
HB4	3.04	-0.22 (-a)	1.26 (+i)	-	4.08	3.89	0.19
HB5	2.81	-0.14(-b)	-0.14(-j)	1.02 (+f)	3.55	3.39	0.16
HB6	2.81	-0.14(-b)	-0.13(-k)	1.03 (+g)	3.58	3.40	0.18
HB7	2.81	-0.14(-b)	-0.14(-l)	1.02 (+h)	3.55	3.39	0.16
HB8	2.81	-0.13(-b)	-0.13(-m)	1.03 (+i)	3.58	3.40	0.18
HB9	2.91	-0.14(-c)	-0.15(-j)	1.03 (+n)	3.64	3.54	0.10
HB10	2.84	-0.15(-c)	1.06 (+o)	-0.15(-k)	3.60	3.46	0.14
HB11	2.91	-0.14(-c)	1.03(+p)	-0.15 (-l)	3.64	3.54	0.10
HB12	2.84	-0.15(-c)	1.06(+q)	-0.15 (-m)	3.60	3.46	0.14
HB13	2.84	-0.13(-d)	-0.34(-r)	0.98 (+n)	3.35	3.40	0.05
HB14	2.81	-0.13(-d)	-0.11(-s)	1.11 (+o)	3.67	3.46	0.21
HB15	2.84	-0.13(-d)	-0.34(-t)	0.98 (+p)	3.35	3.40	0.05
HB16	2.81	-0.13(-d)	-0.11(-u)	1.11 (+q)	3.67	3.46	0.21
HB17	2.73	1.41 (+e)	0.73 (+r)partial	-	4.87	4.81	0.06
HB18	3.04	1.42 (+e)	-0.30 (-s)	-	4.16	3.94	0.22
HB19	2.73	1.41 (+e)	0.73 (+t)partial	-	4.87	4.81	0.06
HB20	3.04	1.42 (+e)	-0.30 (-u)	-	4.16	3.94	0.22
HB21	2.72	1.19 (+f)	1.19 (+i)	-	5.10	4.98	0.12
HB22	2.57	1.10 (+f)	1.10 (+g)	-	4.77	4.88	0.11
HB23	2.72	1.19 (+g)	1.19 (+h)	-	5.10	4.98	0.12
HB24	2.57	1.10 (+i)	1.10(+h)	-	4.77	4.88	0.11
HB25	2.50	-0.13 (-j)	-0.13 (-m)	-	2.24	3.07	0.83
HB26	2.54	-0.16 (-j)	-0.15 (-k)	-	2.23	3.19	0.96
HB27	2.50	-0.13 (-l)	-0.13 (-k)	-	2.24	3.07	0.83
HB28	2.54	-0.16 (-l)	-0.15 (-m)	-	2.23	3.19	0.96
HB29	2.62	0.98 (+n)	1.08 (+q)	-	4.68	5.00	0.32
HB30	2.45	1.03 (+n)	1.08 (+o)	-	4.56	5.08	0.52
HB31	2.62	0.98 (+p)	1.08 (+o)	-	4.68	5.00	032
HB32	2.45	1.03 (+p)	1.08 (+q)	-	4.56	5.08	0.52
HB33	1.88	0.12 (-r)	-0.10 (-u)	-	1.90	2.13	0.23
HB34	2.54	0.27 (-r)	-0.32 (-s)	-	2.49	2.95	0.46
HB35	1.88	0.12 (-t)	-0.10 (-s)	-	1.90	2.13	0.23
HB36	2.54	0.27 (-t)	-0.32 (-u)	-	2.49	2.95	0.46

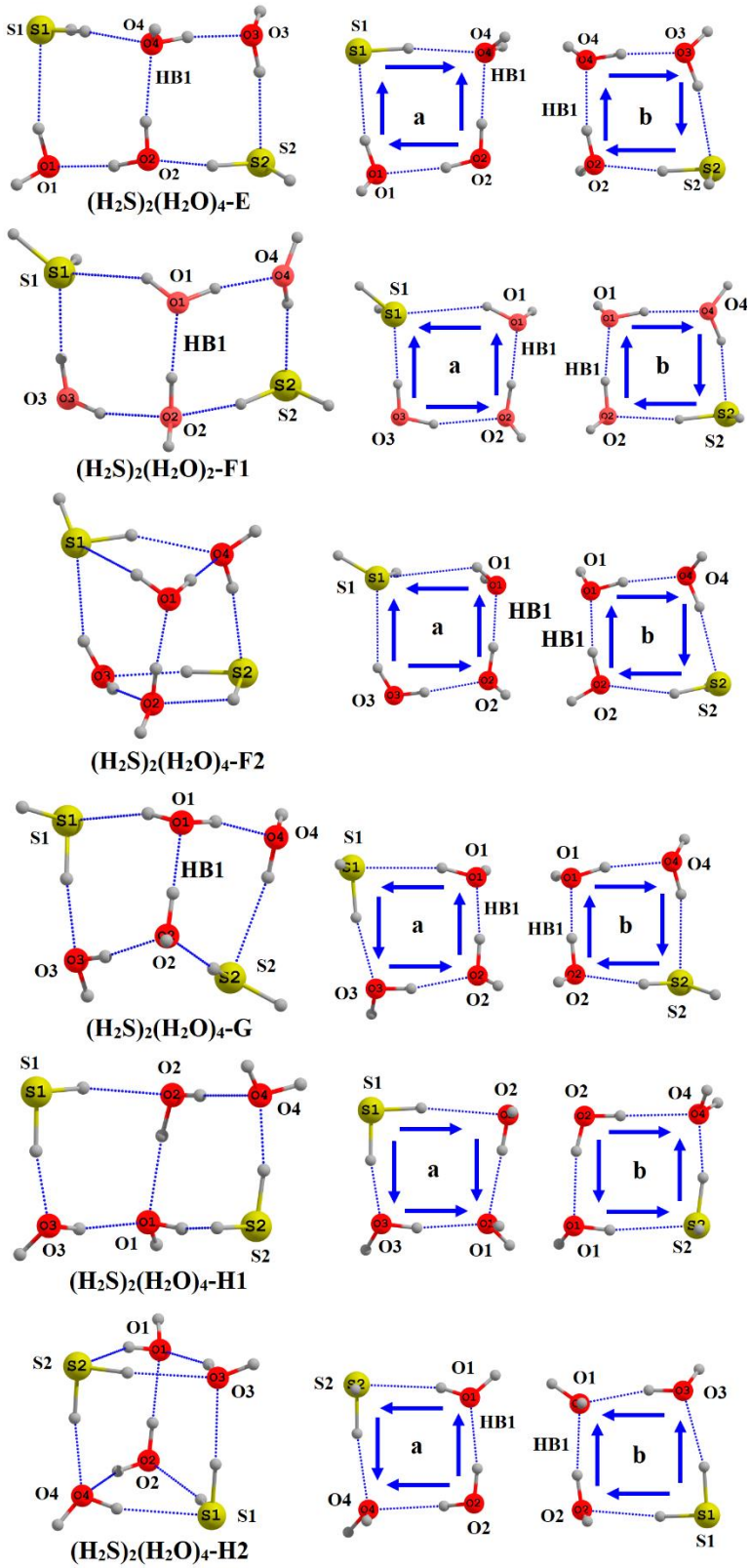


Fig. S2 Structure of $(H_2S)_2(H_2O)_4$ clusters in various possible combinations of two tetrameric cooperative cycles common to O-H…O HBs leading different conformations **E** to **H** of $(H_2S)_2(H_2O)_4$ cluster.

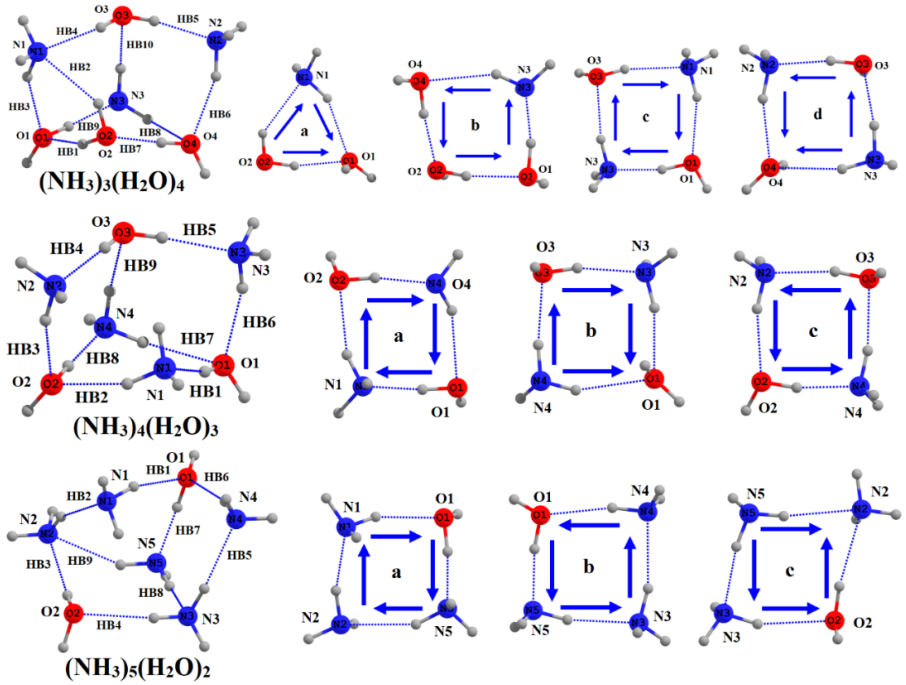


Fig. S3 Structure of **$(NH_3)_3(H_2O)_4$**, **$(NH_3)_4(H_2O)_3$** and **$(NH_3)_5(H_2O)_2$** clusters. The **$(NH_3)_3(H_2O)_4$** consists of one trimeric (a) and three tetrameric cooperative cycles (b to d)). The **$(NH_3)_4(H_2O)_3$** and **$(NH_3)_5(H_2O)_2$** clusters consist of three tetrameric cooperative cycles (a to c).

Table S5 The N-H…O, O-H…N and O-H…O HB energies (in kcal/mol) in **$(NH_3)_3(H_2O)_4$** and **$(NH_3)_4(H_2O)_3$** clusters obtained by synergetic addition of cyclic cooperativity contributions ($E_{HB}^{Synergetic}$) and that by MTA-based method employing actual cluster ($\boldsymbol{E_{HB}^{MTA}}$). The hydrogen bond energy in the respective dimer species (E_{HB}^{Dimer}**)** are also provided (kcal/mol). All the calculations were performed at MP2/aug-cc-pVTZ level of theory. See Fig S3 and text for details.

HB	E_{HB}^{Dimer}	$E_{coop.}^{Cycle1}$	$E_{coop.}^{Cycle2}$	$E_{HB}^{Synergetic}$	$E_{HB}^{(NH_3)_m(H_2O)_n}$	$\lvert\Delta E_{\mathrm{HB}}\rvert$
			$(NH_3)_3(H_2O)_4$			
HB1	4.34	-0.65 (-a)	3.40 (+b)	7.09	7.36	0.27
HB3	2.36	-0.65 (-a)	1.78 (+c)	3.49	3.18	0.31
HB8	2.58	-0.50 (-d)	2.01 (+b)	4.09	4.01	0.08
HB9	6.82	2.21 (+c)	2.93 (+b)	11.96	12.04	0.08
HB10	1.91	1.93 (+c)	0.19 (-d)	4.03	3.85	0.18
			$(NH_3)_4(H_2O)_3$			
HB7	2.57	1.89 (+a)	-0.53 (-b)	3.93	3.80	0.13
HB8	6.90	2.11 (+a)	2.50 (+c)	11.51	11.53	0.02
HB9	2.04	2.29 (+c)	0.19 (-b)	4.52	4.25	0.27
			$(NH_3)_5(H_2O)_2$			
HB7	6.92	1.78 (+a)	2.43 (+b)	11.13	10.89	0.24
HB8	2.75	2.06 (+b)	-0.01 (-c)	4.80	4.50	0.30
HB9	3.13	1.44 (+a)	-0.59 (-c)	3.98	3.89	0.09

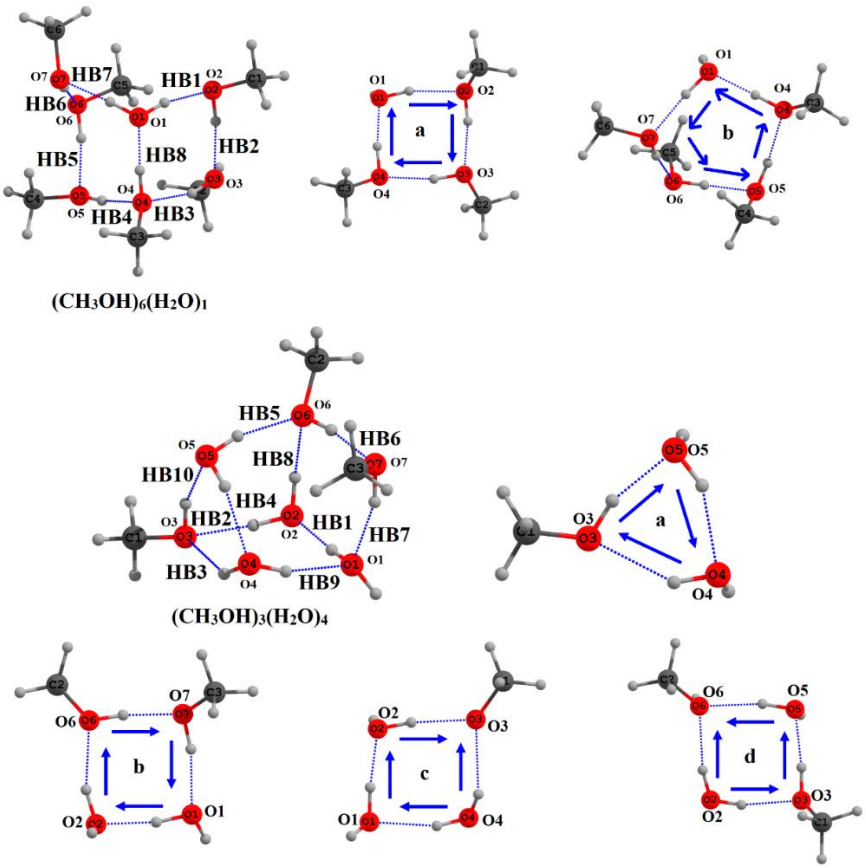


Fig. S4 The MP2 optimized geometries of **$(CH_3OH)_6(H_2O)_1$** and **$(CH_3OH)_3(H_2O)_4$** clusters. See main text for details.

Table S6 The hydrogen bond energies (in kcal/mol) in **$(CH_3OH)_6(H_2O)_1$** and **$(CH_3OH)_3(H_2O)_4$** clusters obtained by synergetic addition of cyclic cooperativity contributions ($E_{HB}^{Synergetic}$) and that by MTA-based method employing actual cluster ($\boldsymbol{E_{HB}^{MTA}}$). The hydrogen bond energy in the respective dimer species (E_{HB}^{Dimer}**)** is also provided (kcal/mol). All the calculations were performed at MP2/aug-cc-pVTZ level of theory. See Fig. S4 and text for details.

HB	$\boldsymbol{E_{HB}^{Dimer}}$	$\boldsymbol{E_{coop.}^{Cycle1}}$	$\boldsymbol{E_{coop.}^{Cycle2}}$	$\boldsymbol{E_{HB}^{Synergetic}}$	$\boldsymbol{E_{HB}^{(CH_3OH)_m(H_2O)_n}}$	$\lvert\Delta E_{\mathrm{HB}}\rvert$
			$(CH_3OH)_6(H_2O)_1$			
HB8	3.80	4.41 (+a)	4.31 (+b)	12.52	12.40	0.12
			$(CH_3OH)_3(H_2O)_4$			
HB1	4.50	3.81 (+b)	2.30 (+c) partial	10.61	10.90	0.29
HB2	4.30	-0.07 (-d)	0.87 (-c)	5.10	5.10	0.00
HB3	4.80	2.20 (+a)	-0.61 (-c)	6.38	6.60	0.22
HB8	5.60	3.49 (+b)	-1.50 (-d)	7.60	7.70	0.10
HB10	4.40	2.31 (+a)	1.94 (+d) partial	8.65	9.10	0.45

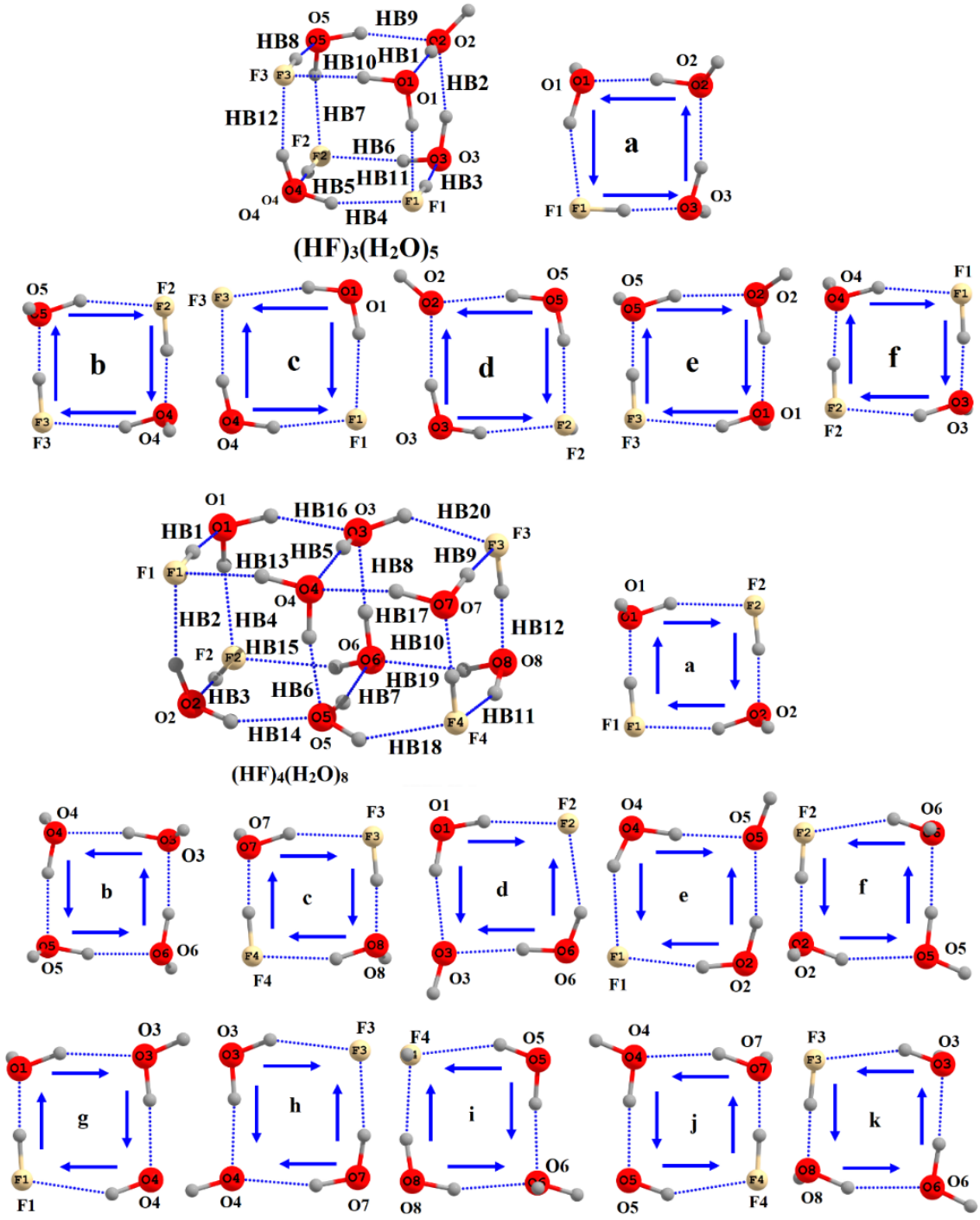


Fig. S5 Structure of $(HF)_3(H_2O)_5$ cluster consisting of six tetrameric cooperative cycles (**a** to **f**) and that of $(HF)_4(H_2O)_8$ cluster with eleven tetrameric cooperative cycles (**a** to **k**).

Table S7 Cartesian coordinates of various molecular clusters optimized at MP2/aug-cc-pVDZ level of theory.

$(NH_3)_8$
E(MP2(full)/ aug-cc-pVTZ) = -451.8966258 a.u.

N	-2.109504000	1.726363000	1.261954000
H	-3.067935000	1.462392000	1.466698000
H	-2.040322000	2.717953000	1.467270000
H	-1.966549000	1.609821000	0.253791000
N	1.125441000	1.375173000	1.703012000
H	1.494154000	1.825752000	2.533881000
H	1.376005000	0.390004000	1.761470000
H	0.110179000	1.426298000	1.761222000
N	2.108586000	-1.726831000	1.262704000
H	2.039121000	-2.718481000	1.467634000
H	3.066912000	-1.463068000	1.468204000
H	1.966354000	-1.609927000	0.254480000
N	-1.126643000	-1.375777000	1.701985000
H	-1.377238000	-0.390629000	1.760664000
H	-1.495891000	-1.826680000	2.532440000
H	-0.111418000	-1.426924000	1.760821000
N	-1.726176000	-2.108774000	-1.263200000
H	-2.717715000	-2.039302000	-1.468666000
H	-1.462345000	-3.067145000	-1.468405000
H	-1.609804000	-1.966380000	-0.254937000
N	1.376054000	-1.125773000	-1.702266000
H	1.427226000	-0.110523000	-1.760647000
H	1.827031000	-1.494655000	-2.532845000
H	0.390907000	-1.376324000	-1.761153000
N	1.727100000	2.109242000	-1.261454000
H	2.718791000	2.039848000	-1.466211000
H	1.609979000	1.966501000	-0.253327000
H	1.463409000	3.067680000	-1.466528000
N	-1.374845000	1.126394000	-1.702733000
H	-0.389667000	1.376983000	-1.760941000
H	-1.825319000	1.495521000	-2.533475000
H	-1.425962000	0.111162000	-1.761451000

$(NH_3)_{20}$
E(MP2/ aug-cc-pVTZ) = -1129.398431 a.u.

N	5.681444000	2.036575000	-1.789984000
H	5.907471000	2.998609000	-1.554437000
H	5.905455000	1.926368000	-2.774748000
H	4.659308000	1.926225000	-1.691446000
N	6.043009000	1.153394000	1.313277000
H	6.101095000	0.137711000	1.401841000
H	6.872650000	1.540293000	1.751668000
H	6.099092000	1.371269000	0.317200000
N	5.681386000	-2.036656000	1.789979000
H	5.907396000	-2.998701000	1.554465000

H	4.659260000	-1.926267000	1.691387000
H	5.905358000	-1.926423000	2.774748000
N	6.042973000	-1.153450000	-1.313281000
H	6.099026000	-1.371308000	-0.317198000
H	6.872614000	-1.540378000	-1.751645000
H	6.101076000	-0.137770000	-1.401861000
N	2.832394000	1.326972000	-1.163257000
H	2.874711000	1.403518000	-0.148037000
H	1.893969000	1.628580000	-1.424760000
H	2.871600000	0.330622000	-1.373218000
N	3.243353000	1.889871000	2.159942000
H	3.115439000	2.894639000	2.075921000
H	3.116779000	1.669069000	3.143924000
H	4.232173000	1.692595000	1.932342000
N	2.832378000	-1.326908000	1.163197000
H	1.893928000	-1.628431000	1.424722000
H	2.874666000	-1.403450000	0.147976000
H	2.871676000	-0.330560000	1.373144000
N	3.243309000	-1.889997000	-2.159859000
H	3.116786000	-1.669571000	-3.143932000
H	3.115348000	-2.894726000	-2.075454000
H	4.232130000	-1.692677000	-1.932300000
N	-0.272480000	2.198121000	-1.890660000
H	-0.127847000	3.173993000	-1.645901000
H	-0.122904000	2.134042000	-2.894016000
H	-1.271847000	1.992514000	-1.725290000
N	0.147102000	1.146749000	1.302395000
H	0.101739000	0.132694000	1.392741000
H	1.084536000	1.410094000	1.606917000
H	0.114638000	1.348582000	0.303912000
N	-0.272294000	-2.197944000	1.890728000
H	-0.127616000	-3.173856000	1.646155000
H	-1.271655000	-1.992392000	1.725250000
H	-0.122804000	-2.133687000	2.894086000
N	0.147042000	-1.146532000	-1.302490000
H	0.114692000	-1.348449000	-0.304021000
H	1.084481000	-1.409718000	-1.607127000
H	0.101520000	-0.132477000	-1.392762000
N	-3.049451000	1.280937000	-1.195478000
H	-3.066928000	1.349219000	-0.179371000
H	-3.984813000	1.537923000	-1.505734000
H	-2.944701000	0.291817000	-1.418808000
N	-2.607932000	1.930546000	2.140332000
H	-2.780914000	2.909939000	1.929968000
H	-2.715644000	1.833108000	3.146469000
H	-1.610229000	1.750679000	1.931583000
N	-3.049269000	-1.280926000	1.195358000
H	-3.984596000	-1.537973000	1.505666000
H	-3.066785000	-1.349244000	0.179254000
H	-2.944572000	-0.291797000	1.418667000

N	-2.607922000	-1.930458000	-2.140515000
H	-2.715632000	-1.832824000	-3.146633000
H	-2.780857000	-2.909902000	-1.930348000
H	-1.610232000	-1.750577000	-1.931721000
N	-6.312978000	1.987946000	-1.140011000
H	-6.198002000	1.770951000	-0.137399000
H	-6.048047000	2.958585000	-1.279163000
H	-7.304156000	1.929242000	-1.354116000
N	-5.712653000	1.081060000	1.681273000
H	-6.180412000	1.405026000	2.521813000
H	-4.716808000	1.274080000	1.794056000
H	-5.820933000	0.064454000	1.644998000
N	-6.312890000	-1.988071000	1.140186000
H	-6.197975000	-1.771089000	0.137565000
H	-7.304061000	-1.929444000	1.354337000
H	-6.047867000	-2.958685000	1.279349000
N	-5.712718000	-1.081227000	-1.681152000
H	-5.820967000	-0.064619000	-1.644860000
H	-4.716888000	-1.274273000	-1.794029000
H	-6.180565000	-1.405174000	-2.521651000

$(H_2S)_8$
MP2(full)/aug-cc-pVTZ= -3191.6419771 a.u.

S	2.394462000	-2.150190000	2.137413000
H	2.480478000	-0.798877000	2.120198000
H	1.053066000	-2.105273000	2.317209000
S	1.560585000	1.733776000	1.723687000
H	1.906148000	1.984707000	0.433848000
H	2.378156000	2.693279000	2.206753000
S	2.446809000	2.134988000	-2.096767000
H	2.529793000	0.783478000	-2.079316000
H	1.108224000	2.092944000	-2.297683000
S	1.579641000	-1.742721000	-1.699379000
H	2.395898000	-2.711075000	-2.166770000
H	1.900037000	-1.995487000	-0.403435000
S	-1.592469000	-1.704312000	1.729002000
H	-2.421633000	-2.175934000	2.684235000
H	-1.923203000	-0.409940000	1.976482000
S	-2.432597000	2.128328000	2.119097000
H	-1.091270000	2.312397000	2.090998000
H	-2.501068000	2.107232000	0.766816000
S	-1.548608000	1.714122000	-1.753690000
H	-2.358469000	2.189592000	-2.723464000
H	-1.882507000	0.421466000	-2.005846000
S	-2.408023000	-2.113303000	-2.159643000
H	-2.501780000	-2.093013000	-0.808890000
H	-1.068663000	-2.306495000	-2.106648000

$(H_2O)_4(H_2S)_2$-A
MP2(full)/aug-cc-pVTZ = -1103.3292035 a.u.

O	2.802707000	-0.906395000	-0.929588000
H	2.186157000	-1.283345000	-0.273320000
H	2.688979000	-1.459735000	-1.713089000
O	2.058191000	1.797873000	-1.056680000
H	2.375493000	0.870844000	-1.062023000
H	2.840832000	2.318745000	-0.836572000
S	-0.615293000	2.183187000	0.908903000
H	-0.326796000	1.092970000	1.653987000
H	0.479541000	2.018952000	0.110271000
O	-2.735324000	0.524403000	-1.069952000
H	-2.129891000	1.065515000	-0.524997000
H	-3.617735000	0.782581000	-0.774058000
O	-1.901255000	-2.119704000	-0.922570000
H	-2.256758000	-1.208867000	-1.012381000
H	-1.788419000	-2.424583000	-1.831437000
S	0.468481000	-1.638514000	1.336050000
H	-0.486595000	-1.945026000	0.409350000
H	0.589629000	-2.912228000	1.765351000

$(H_2O)_4(H_2S)_2$-B
MP2(full)/aug-cc-pVTZ = -1103.320266 a.u.

S	0.231254000	-1.688134000	1.238505000
H	-0.670965000	-1.894226000	0.245701000
H	1.276241000	-1.586889000	0.387167000
S	-0.448717000	1.992240000	0.417414000
H	-0.201473000	0.720858000	0.840704000
H	-0.520527000	2.473591000	1.674850000
O	3.159584000	-1.172311000	-0.774598000
H	3.239149000	-1.408405000	-1.708373000
H	3.996358000	-1.458480000	-0.384594000
O	2.954900000	1.787205000	-0.589747000
H	2.064561000	2.013807000	-0.285484000
H	2.955230000	0.817062000	-0.605610000
O	-2.284753000	-1.804086000	-1.010816000
H	-2.739929000	-0.942281000	-0.928114000
H	-2.541599000	-2.138718000	-1.877841000
O	-3.405791000	0.746212000	-0.588203000
H	-2.667492000	1.266810000	-0.223850000
H	-4.101662000	0.815015000	0.077657000

$(H_2O)_4(H_2S)_2$-C
MP2(full)/aug-cc-pVTZ = -1103.325805 a.u.

S	-0.055955000	1.809484000	1.173572000
H	0.900220000	1.853175000	0.210713000
H	-1.082725000	1.764758000	0.286048000
S	0.100115000	-1.875724000	0.574315000
H	0.043475000	-0.546403000	0.902358000

H	0.036373000	-2.276757000	1.860086000
O	-2.725396000	1.369156000	-0.927948000
H	-3.557318000	1.829070000	-0.762924000
H	-2.942293000	0.421743000	-0.826555000
O	-3.058735000	-1.426712000	-0.575097000
H	-2.202154000	-1.711323000	-0.211223000
H	-3.173075000	-1.968297000	-1.366418000
O	2.531770000	1.534302000	-1.023021000
H	2.814464000	0.601646000	-0.954985000
H	2.572015000	1.735656000	-1.965512000
O	3.192663000	-1.192735000	-0.598917000
H	2.423199000	-1.558260000	-0.129384000
H	3.938841000	-1.357258000	-0.008520000

$(H_2O)_4(H_2S)_2$-D1
MP2(full)/aug-cc-pVTZ = -1103.3145399 a.u.

O	-3.088847000	-1.189663000	-1.021912000
H	-3.981569000	-1.538022000	-0.896757000
H	-2.759881000	-1.645777000	-1.808848000
O	-2.396415000	1.916236000	-0.575404000
H	-2.662868000	1.004271000	-0.781281000
H	-2.779765000	2.442387000	-1.288749000
S	0.819019000	2.256109000	0.716127000
H	0.567082000	1.245430000	1.576533000
H	-0.405285000	2.150451000	0.139432000
O	2.809158000	0.377464000	-1.371511000
H	2.255892000	0.958645000	-0.818692000
H	3.713791000	0.641734000	-1.159239000
O	2.245423000	-2.317264000	-0.665150000
H	2.455069000	-1.408583000	-0.945887000
H	1.456067000	-2.206795000	-0.118273000
S	-0.332973000	-1.499275000	1.327224000
H	-0.754170000	-2.629400000	1.933247000
H	-1.435648000	-1.417876000	0.546723000

$(H_2O)_4(H_2S)_2$-D2
MP2(full)/aug-cc-pVTZ = -1103.3397101 a.u.

S	-1.636341000	1.915087000	-0.030915000
H	-1.656124000	0.847885000	-0.866363000
H	-2.179232000	2.746876000	-0.944463000
S	2.341590000	1.365952000	-0.012187000
H	1.075553000	1.830825000	-0.136261000
H	2.110711000	0.349325000	-0.875711000
O	-1.725535000	-1.251704000	1.451115000
H	-2.246418000	-0.481897000	1.715704000
H	-1.823595000	-1.291507000	0.477874000
O	1.060732000	-1.452746000	1.480513000
H	0.101296000	-1.325744000	1.644637000
H	1.436791000	-0.557449000	1.505482000
O	-1.510113000	-1.258634000	-1.357223000

H	-0.575655000	-1.566198000	-1.438111000
H	-2.014828000	-1.802102000	-1.974738000
O	1.142212000	-1.874690000	-1.176248000
H	1.566555000	-2.706832000	-1.419817000
H	1.182611000	-1.837622000	-0.183858000

$(H_2O)_4(H_2S)_2$-E
MP2(full)/aug-cc-pVTZ = -1103.3338019 a.u.

S	3.115082000	-0.684154000	-0.626977000
H	2.041649000	-1.113632000	0.088127000
H	2.435679000	-0.709433000	-1.793815000
O	1.903173000	2.416905000	-0.030814000
H	2.428571000	1.615877000	-0.210828000
H	2.506047000	3.001890000	0.445803000
O	-0.417493000	1.260610000	1.193003000
H	-0.087362000	0.352307000	1.320050000
H	0.344431000	1.742451000	0.818033000
S	-3.050554000	0.812026000	-0.649541000
H	-1.951498000	1.115308000	0.117017000
H	-3.886362000	0.820399000	0.410899000
O	-1.902122000	-2.247293000	-0.169243000
H	-2.352918000	-1.402023000	-0.374911000
H	-1.905926000	-2.735492000	-1.002434000
O	0.348906000	-1.532017000	1.234179000
H	-0.425945000	-1.877883000	0.734893000
H	0.361480000	-2.041357000	2.054440000

$(H_2O)_4(H_2S)_2$-F1
MP2(full)/aug-cc-pVTZ = -1103.3162089 a.u.

O	-0.141119000	1.391412000	1.470296000
H	0.593703000	1.727235000	0.911541000
H	-0.938101000	1.586691000	0.957244000
O	0.339425000	-1.295613000	1.487424000
H	0.133738000	-0.336109000	1.601398000
H	0.427603000	-1.645294000	2.383069000
S	-2.838704000	0.639743000	-0.594836000
H	-2.528857000	0.550329000	-1.904879000
H	-4.052345000	1.182577000	-0.826982000
O	-1.974613000	-2.098108000	-0.201486000
H	-1.199763000	-2.029396000	0.382599000
H	-2.336937000	-1.203706000	-0.204421000
O	2.022006000	2.024011000	-0.124570000
H	2.286700000	1.223942000	-0.619532000
H	2.132521000	2.769371000	-0.728160000
S	2.712013000	-0.779030000	-0.852261000
H	1.813325000	-1.102357000	0.119878000
H	3.729886000	-0.668297000	0.028495000

$(H_2O)_4(H_2S)_2$-F2
MP2(full)/aug-cc-pVTZ = -1103.3358741 a.u.

O	1.781832000	-1.325290000	1.432385000
H	1.553946000	-1.698455000	0.550331000
H	2.217581000	-2.040312000	1.912259000
O	-0.786149000	-0.324105000	2.023864000
H	0.139257000	-0.636655000	1.961010000
H	-0.739314000	0.639417000	1.916698000
S	1.865206000	1.399783000	-0.828248000
H	2.177466000	0.708763000	0.293460000
H	0.671285000	1.796385000	-0.324114000
O	-1.285793000	2.211323000	0.606610000
H	-1.689360000	3.082027000	0.717327000
H	-1.932602000	1.698134000	0.093342000
O	1.031713000	-1.878972000	-1.166027000
H	0.067005000	-1.942499000	-1.257704000
H	1.221268000	-0.965317000	-1.446151000
S	-2.158379000	-0.656046000	-0.886526000
H	-1.643134000	-0.691405000	0.388151000
H	-3.285448000	-1.313537000	-0.542887000

$(H_2O)_4(H_2S)_2$-G
MP2(full)/aug-cc-pVTZ = -1103.3366492 a.u.

O	0.517683000	-1.459843000	1.466682000
H	-0.107010000	-1.954790000	0.897996000
H	1.274557000	-1.281090000	0.880130000
O	-0.598481000	0.935634000	1.936028000
H	-0.181909000	0.035581000	1.867713000
H	-0.652831000	1.127703000	2.880112000
S	2.743608000	-0.324029000	-0.843380000
H	3.761011000	0.056441000	-0.041863000
H	2.045508000	0.825503000	-0.626154000
O	0.852709000	2.327773000	-0.018179000
H	0.335849000	1.969078000	0.732108000
H	0.209978000	2.820604000	-0.544427000
O	-1.446763000	-2.522089000	-0.254304000
H	-1.776183000	-1.695092000	-0.651393000
H	-1.265931000	-3.101899000	-1.005391000
S	-2.292267000	0.668672000	-0.976273000
H	-1.871752000	0.826976000	0.306054000
H	-3.593927000	0.604893000	-0.622268000

$(H_2O)_4(H_2S)_2$-H1
MP2(full)/aug-cc-pVTZ = -1103.3103171 a.u.

O	-0.104475000	-1.552857000	1.367067000
H	-0.931237000	-1.461054000	0.851361000
H	-0.349272000	-2.085219000	2.135601000
O	0.046945000	1.400748000	1.694656000
H	0.068796000	0.429486000	1.707095000
H	-0.625600000	1.604581000	1.027164000
O	1.952689000	-1.979700000	-0.572728000
H	1.315165000	-1.956049000	0.166894000

H	2.459294000	-2.790674000	-0.435198000
S	2.933552000	0.943581000	-0.552796000
H	2.629067000	-0.371931000	-0.613690000
H	1.984794000	1.200025000	0.377823000
S	-2.687300000	-0.863269000	-0.583181000
H	-2.563610000	0.430780000	-0.572068000
H	-1.902040000	-0.999967000	-1.673220000
O	-2.075396000	2.069067000	-0.442369000
H	-2.898182000	2.506339000	-0.114322000
H	-1.685310000	2.710632000	-1.054807000

$(H_2O)_4(H_2S)_2$-H2
MP2(full)/aug-cc-pVTZ = -1103.3327729 a.u.

O	-1.381910000	-1.149339000	1.627614000
H	-1.907484000	-0.508667000	1.105366000
H	-1.976402000	-1.453620000	2.325993000
O	1.054687000	0.444759000	2.201589000
H	0.249267000	-0.096941000	2.145211000
H	0.835961000	1.231156000	1.674725000
O	-0.483083000	-2.164657000	-0.887752000
H	-0.737711000	-2.090987000	0.051257000
H	-0.387385000	-3.112511000	-1.045940000
S	2.543374000	-0.384216000	-0.782025000
H	1.403364000	-1.086546000	-1.004142000
H	2.275798000	-0.297038000	0.548259000
S	-2.404760000	0.783989000	-0.803388000
H	-1.249529000	1.472179000	-0.610677000
H	-1.762566000	-0.252888000	-1.392748000
O	0.656983000	2.249642000	-0.130029000
H	0.974133000	3.127459000	-0.380011000
H	1.291324000	1.628791000	-0.542067000

$(NH_3)_3(H_2O)_4$
MP2/aug-cc-pVTZ = -474.7813386 a.u.

O	2.417835000	-1.068158000	0.366655000
H	1.657415000	-1.102563000	1.027973000
H	3.012217000	-1.788809000	0.607747000
O	0.567587000	-0.711722000	-1.687254000
H	1.289395000	-1.003041000	-1.090504000
H	0.601448000	0.252497000	-1.577253000
N	2.013556000	1.818500000	-0.694532000
H	2.456651000	1.009327000	-0.247927000
H	2.491773000	1.957187000	-1.585445000
H	2.248809000	2.631178000	-0.122874000
O	-0.492572000	1.852769000	0.923203000
H	-1.354965000	1.654888000	0.492478000
H	0.152708000	1.877006000	0.194577000
N	-2.992363000	0.942941000	-0.185283000
H	-2.773791000	-0.046344000	-0.341783000
H	-3.384191000	1.303283000	-1.054942000

H	-3.744678000	0.978040000	0.502274000
O	-1.679380000	-1.809762000	-0.556422000
H	-1.925080000	-2.587653000	-1.071689000
H	-0.893504000	-1.438729000	-1.025460000
N	0.156594000	-0.937319000	1.869596000
H	-0.100204000	0.050692000	1.734731000
H	0.081390000	-1.138662000	2.865600000
H	-0.567666000	-1.482164000	1.394566000

$(NH_3)_4(H_2O)_3$
MP2/aug-cc-pVTZ = -454.9095725 a.u.

O	-2.195760000	-1.628673000	-0.176304000
H	-2.612999000	-2.411191000	-0.556516000
H	-1.474799000	-1.379272000	-0.815348000
N	-0.099868000	-0.621191000	-1.709881000
H	0.781736000	-1.046400000	-1.405140000
H	-0.062299000	0.349604000	-1.392969000
H	-0.088755000	-0.596081000	-2.729075000
O	2.289097000	-1.449835000	-0.022619000
H	1.596368000	-1.404502000	0.703802000
H	2.849235000	-2.201637000	0.204116000
N	2.386660000	1.563471000	-0.591187000
H	2.583089000	0.570890000	-0.423176000
H	2.573306000	1.739685000	-1.578270000
H	3.088763000	2.092723000	-0.073793000
O	-0.008651000	1.856905000	1.054390000
H	-0.840037000	1.828199000	0.535535000
H	0.717968000	1.880155000	0.397898000
N	-2.620351000	1.431629000	-0.165842000
H	-2.722782000	0.412415000	-0.128232000
H	-2.984061000	1.730328000	-1.070684000
H	-3.256357000	1.816619000	0.532828000
N	0.243710000	-1.060883000	1.764734000
H	0.132160000	-0.038589000	1.706031000
H	0.300002000	-1.299908000	2.753964000
H	-0.629089000	-1.461398000	1.410531000

$(NH_3)_5(H_2O)_2$
MP2/aug-cc-pVTZ = -435.019067 a.u.

O	1.462423000	-1.997307000	0.267803000
H	0.854945000	-1.579697000	0.946229000
H	1.637937000	-2.886908000	0.596612000
N	-0.310308000	-0.565365000	-1.847471000
H	0.368690000	-1.136993000	-1.335457000
H	-0.168666000	0.396036000	-1.530813000
H	-0.034166000	-0.589646000	-2.828879000
N	-2.740407000	-1.262992000	-0.037322000
H	-2.652829000	-2.207393000	0.340903000
H	-2.049338000	-1.191798000	-0.797767000
H	-3.662945000	-1.229099000	-0.472881000

O	-2.061477000	1.916108000	-0.539755000
H	-2.316661000	1.003020000	-0.151847000
H	-2.634905000	2.605253000	-0.052492000
N	0.826033000	2.104113000	0.910016000
H	0.014696000	2.250361000	0.301181000
H	1.590242000	1.748062000	0.324319000
H	1.113634000	3.023468000	1.243396000
N	3.079968000	0.458485000	-0.689855000
H	2.705582000	-0.440270000	-0.368774000
H	3.169410000	0.390192000	-1.703682000
H	4.031380000	0.522949000	-0.327745000
N	-0.248015000	-0.594683000	1.914879000
H	0.103790000	0.367327000	1.792856000
H	-0.332243000	-0.755867000	2.918135000
H	-1.197020000	-0.616311000	1.530592000

$(CH_3OH)_6(H_2O)_1$
MP2/aug-cc-pVTZ = -769.6056432 a.u.

O	-0.298636000	-0.869381000	-1.539193000
H	-0.577721000	-1.519584000	-0.855680000
H	-0.879074000	-0.083238000	-1.397410000
O	-0.687686000	-2.623146000	0.568126000
H	0.203076000	-2.458130000	0.959022000
C	-0.785929000	-4.025605000	0.276995000
H	-0.724943000	-4.627976000	1.197759000
H	0.004460000	-4.351625000	-0.419596000
H	-1.764662000	-4.192644000	-0.192235000
O	1.826407000	-2.000591000	1.399548000
H	2.112059000	-1.464396000	0.627562000
C	2.065598000	-1.217611000	2.583128000
H	1.514289000	-1.693000000	3.405408000
H	3.138363000	-1.205161000	2.833187000
H	1.713147000	-0.181276000	2.460091000
O	2.116209000	-0.311853000	-0.740844000
H	1.202656000	-0.511226000	-1.119007000
C	3.065706000	-0.266251000	-1.820618000
H	2.771945000	0.486660000	-2.569198000
H	3.150680000	-1.248895000	-2.310318000
H	4.039735000	0.009641000	-1.394625000
O	1.601318000	1.868638000	0.818616000
H	1.851487000	1.096378000	0.260658000
C	1.452911000	2.990444000	-0.074582000
H	2.415366000	3.247618000	-0.545358000
H	1.114685000	3.842359000	0.529824000
H	0.702325000	2.785263000	-0.856151000
O	-0.995457000	1.642391000	1.582434000
H	-0.021039000	1.666261000	1.424881000
C	-1.302926000	0.436934000	2.306063000
H	-2.385848000	0.440108000	2.489898000
H	-0.784049000	0.418570000	3.277980000

H	-1.043944000	-0.467112000	1.731827000
O	-1.775326000	1.363708000	-0.991538000
H	-1.543187000	1.524509000	-0.043341000
C	-3.201552000	1.226485000	-1.069574000
H	-3.559000000	0.362513000	-0.482833000
H	-3.458333000	1.067886000	-2.125552000
H	-3.707594000	2.138196000	-0.712924000

$(CH_3OH)_3(H_2O)_4$
MP2/aug-cc-pVTZ = -652.0030525 a.u.

O	0.780267000	1.791335000	1.658708000
H	0.191469000	1.011794000	1.871161000
H	0.849393000	2.306119000	2.472046000
O	-0.728657000	-0.382208000	1.890830000
H	-1.517108000	-0.236821000	1.323920000
H	-0.190247000	-1.016353000	1.375277000
O	-2.681098000	0.130834000	-0.046376000
H	-2.124331000	-0.260183000	-0.765027000
C	-4.010924000	-0.403547000	-0.140401000
H	-4.604555000	0.058139000	0.659451000
H	-4.014113000	-1.497104000	-0.002325000
H	-4.467958000	-0.159549000	-1.112496000
O	-0.659604000	2.137992000	-0.814973000
H	-1.548747000	1.886072000	-0.512902000
H	-0.162248000	2.229881000	0.018745000
O	-0.757756000	-0.544389000	-1.821725000
H	-0.481371000	0.385029000	-1.694779000
H	-0.117989000	-1.049275000	-1.279512000
O	1.009856000	-1.684080000	0.072731000
H	1.698798000	-0.969750000	0.101920000
C	1.673060000	-2.959957000	0.053588000
H	2.283672000	-3.075553000	-0.856175000
H	0.893886000	-3.733252000	0.061220000
H	2.313571000	-3.085596000	0.940669000
C	2.797025000	1.111891000	-1.065624000
H	2.153325000	0.991577000	0.794873000
O	2.665255000	0.413495000	0.189346000
H	3.471205000	1.976008000	-0.960237000
H	1.819822000	1.454738000	-1.440388000
H	3.234770000	0.405488000	-1.783034000

$(HF)_3(H_2O)_5$
E(MP2/ aug-cc-pVTZ) = -682.7973725 a.u.

O	1.841245000	-0.002124000	1.510673000
H	1.267501000	0.763727000	1.686548000
H	1.266548000	-0.767562000	1.685252000
O	2.147804000	-0.000242000	-1.140203000
H	2.196807000	-0.001008000	-0.145793000
H	3.058590000	-0.000494000	-1.460611000
O	0.122117000	-1.919951000	-1.185095000

H	0.905412000	-1.352310000	-1.344874000
H	-0.628813000	-1.398292000	-1.523877000
O	-2.074656000	0.000366000	0.985786000
H	-1.557520000	-0.770521000	1.288251000
H	-1.556688000	0.770241000	1.289410000
O	0.124146000	1.921672000	-1.182168000
H	0.906823000	1.353430000	-1.342830000
H	-0.627349000	1.401362000	-1.521766000
F	-0.175475000	-2.032110000	1.258180000
H	-0.048615000	-2.053194000	0.271601000
F	-1.919318000	0.002124000	-1.468891000
H	-2.052359000	0.001464000	-0.480562000
F	-0.173399000	2.030432000	1.261281000
H	-0.046458000	2.052874000	0.274749000

$(HF)_4(H_2O)_8$

E(MP2/ aug-cc-pVTZ) = -1012.201323 a.u.

O	2.794865000	1.773670000	-0.429186000
H	2.949750000	1.437444000	0.473393000
H	1.880975000	2.119535000	-0.405634000
F	2.848815000	-0.200709000	-1.913872000
H	2.859279000	0.623045000	-1.361616000
O	2.794903000	-1.773668000	0.429160000
H	1.881015000	-2.119534000	0.405624000
H	2.949780000	-1.437433000	-0.473418000
F	2.848835000	0.200712000	1.913844000
H	2.859310000	-0.623043000	1.361586000
O	0.004651000	1.907473000	-0.364706000
H	-0.868773000	2.332746000	-0.394329000
H	-0.062910000	1.161949000	-1.007199000
O	-0.004682000	-0.364683000	-1.907465000
H	0.868744000	-0.394324000	-2.332731000
H	0.062872000	-1.007143000	-1.161909000
O	0.004665000	-1.907467000	0.364697000
H	-0.062893000	-1.161938000	1.007186000
H	-0.868758000	-2.332741000	0.394328000
O	-0.004647000	0.364687000	1.907432000
H	0.868775000	0.394262000	2.332709000
H	0.062890000	1.007196000	1.161924000
F	-2.848851000	1.913862000	-0.200712000
H	-2.859281000	1.361615000	0.623056000
O	-2.794900000	-0.429190000	-1.773623000
H	-2.949786000	0.473389000	-1.437398000
H	-1.881021000	-0.405649000	-2.119511000
F	-2.848835000	-1.913849000	0.200755000
H	-2.859308000	-1.361642000	-0.623036000
O	-2.794848000	0.429199000	1.773681000
H	-2.949737000	-0.473383000	1.437459000
H	-1.880954000	0.405651000	2.119531000