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Electronic Supplemental Information for

Hydration Motifs of Ammonium Bisulfate Clusters of Relevance to Atmospheric New Particle Formation

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Contents

Notes for naming scheme

1Wa - one water cyclic, staggered - 3734
1Wb - one water on SOH, staggered - 3732
1Wc - one water cyclic, eclipsed - 10405
1Wd - one water insertion, staggered - 3733

2Wa - two water opposite sides, near, staggered - 10447
2Wb - two water opposite sides, far, staggered - 10446
2Wc - two water same side, staggered - 10410
2Wd - two water same side, eclipsed - 10622
2We - two water opposite sides, eclipsed - 10411
2Wf - two water on same ammonium, staggered - 10417

3Wa - three water opposite sides, staggered - 10574
3Wb - three water same side, staggered - 10415
3Wc - three water opposite sides, eclipsed - 10425
3Wd - three water same side, eclipsed - 10433
3We - three water one free NH2, staggered - 10573

4Wa - four water opposite sides, fourth water on 2W side - 10633
4Wb - four water same side - 10590
4Wc - four water opposite sides, fourth water on 2W side isomer - 10639
4Wd - four water opposite sides, fourth water on 1W side - 10632
4We - four water insertion - 10594
4Wf - four water, fourth water on opposite SOH - 10592
4Wg - four water all on NH - 10591

Table S1. Zero-point corrected energies and relative energies of the computed clusters

Name of the cluster	Zero-point corrected energy (Hartree)	Energy difference to the lowest energy isomer (kJ/mol)
1Wa	-1647.008678	0
1Wb	-1647.007506	3.1
1Wc	-1647.006432	5.9
1Wd	-1647.005422	8.5
2Wa	-1723.449624	0
2Wb	-1723.449132	1.3
2Wc	-1723.448955	1.8
2Wd	-1723.447135	6.5
2We	-1723.446563	8.0
2Wf	-1723.445143	11.8
3Wa	-1799.889380	0
3Wb	-1799.887779	4.2
3Wc	-1799.886798	6.8
3Wd	-1799.885902	9.1
3We	-1799.884345	13.2
4Wa	-1876.328865	0
4Wb	-1876.328128	1.9
4Wc	-1876.328006	2.3
4Wd	-1876.327241	4.3
4We	-1876.325851	7.9
4Wf	-1876.325657	8.4
4Wg	-1876.325382	9.1

Table S2. Water binding energies of the computed clusters

Zero-point corrected energy: (3,2): -1570.549791 Hartree; H_2O: -76.423419 Hartree.

Name of the cluster	Water binding energy (kJ/mol)	Precursor
1Wa	92	(3,2)
1Wb	89	(3,2)
1Wc	86	(3,2)
1Wd	84	(3,2)
2Wa	46	1Wa
2Wb	44	1Wa
2Wc	44	1Wa
2Wd	45	1Wc
2We	43	1Wc
2Wf	34	1Wa
3Wa	42	2Wa
3Wb	40	2Wc
3Wc	42	2Wd
3Wd	40	2Wd
3We	31	2Wc
4Wa	42	3Wa
4Wb	44	3Wb
4Wc	40	3Wa
4Wd	38	3Wa
4We	34	3Wa
4Wf	38	3Wb
4Wg	33	3Wa

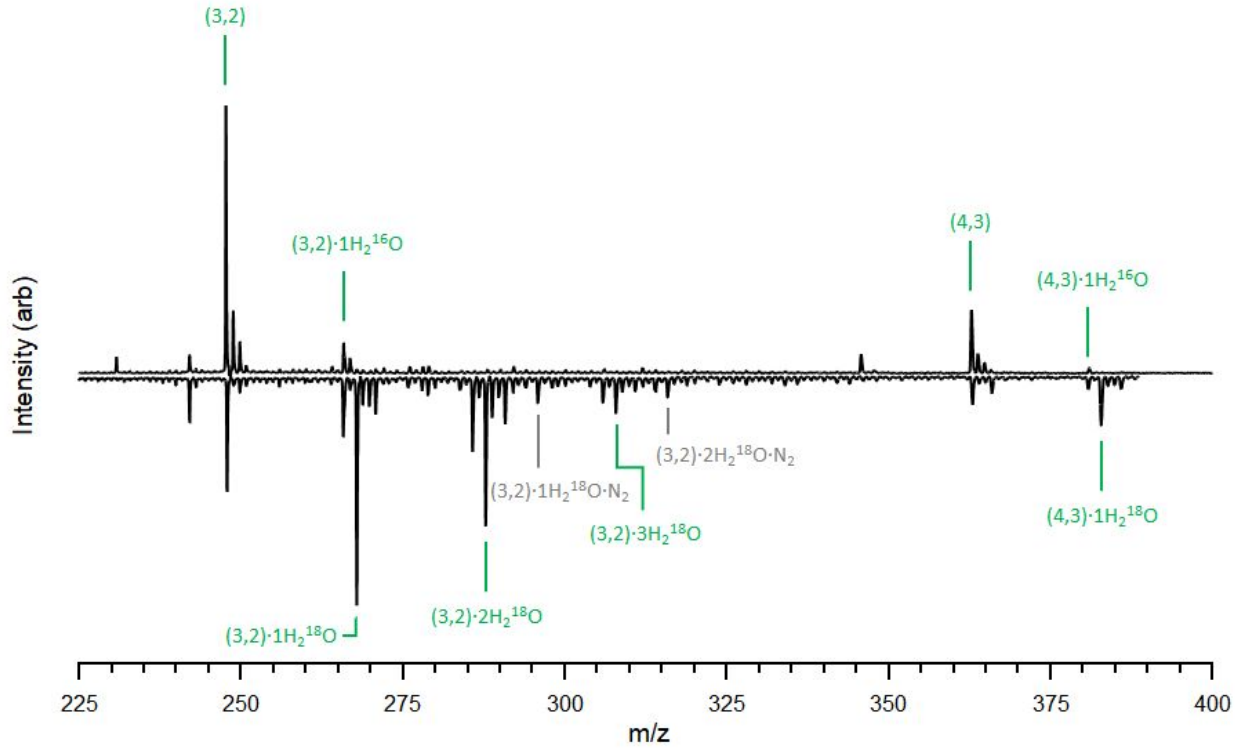


Figure S1. Mass spectra showing hydration and N_2 tagging of (3,2) cluster. On top is the mass spectrum taken with the tagging trap at 20 K and the hydration trap at 190 K, prior to injection of $H_2{}^{18}O$. At the bottom is the mass spectrum after injection of $H_2{}^{18}O$ and with the tagging trap at 23 K.

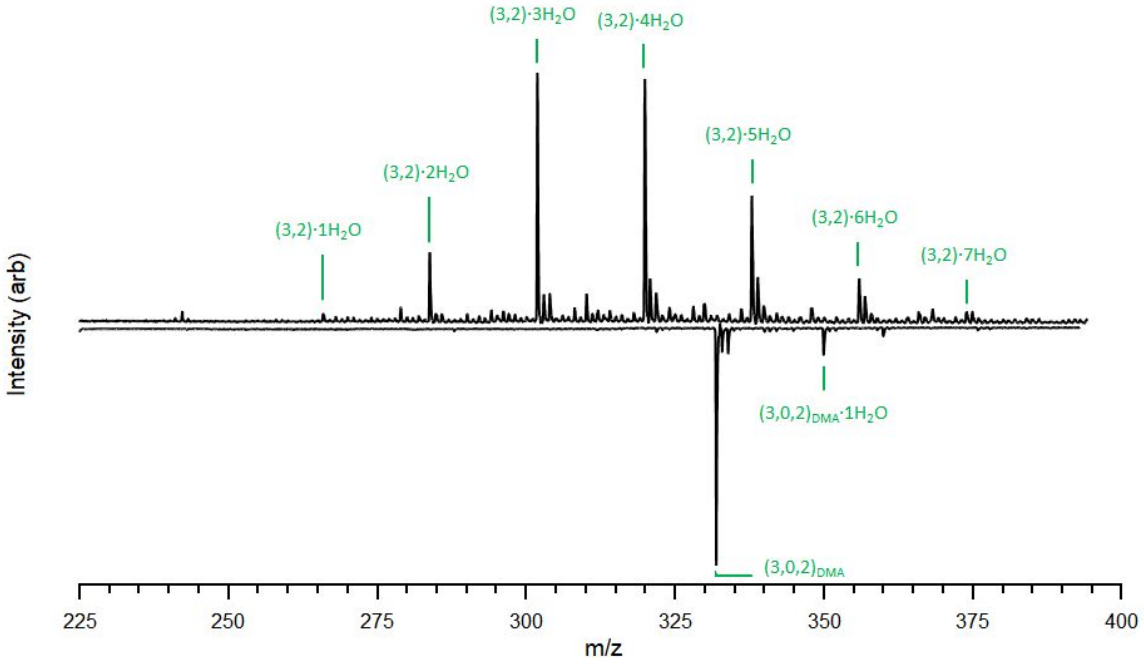


Figure S2. Comparison between mass spectra of hydrated (3,2) (shown at top) and $(3,0,2)_{DMA}$ clusters (shown at bottom). The hydration trap was held at 165 K for both the (3,2) clusters and the $(3,0,2)_{DMA}$ clusters.

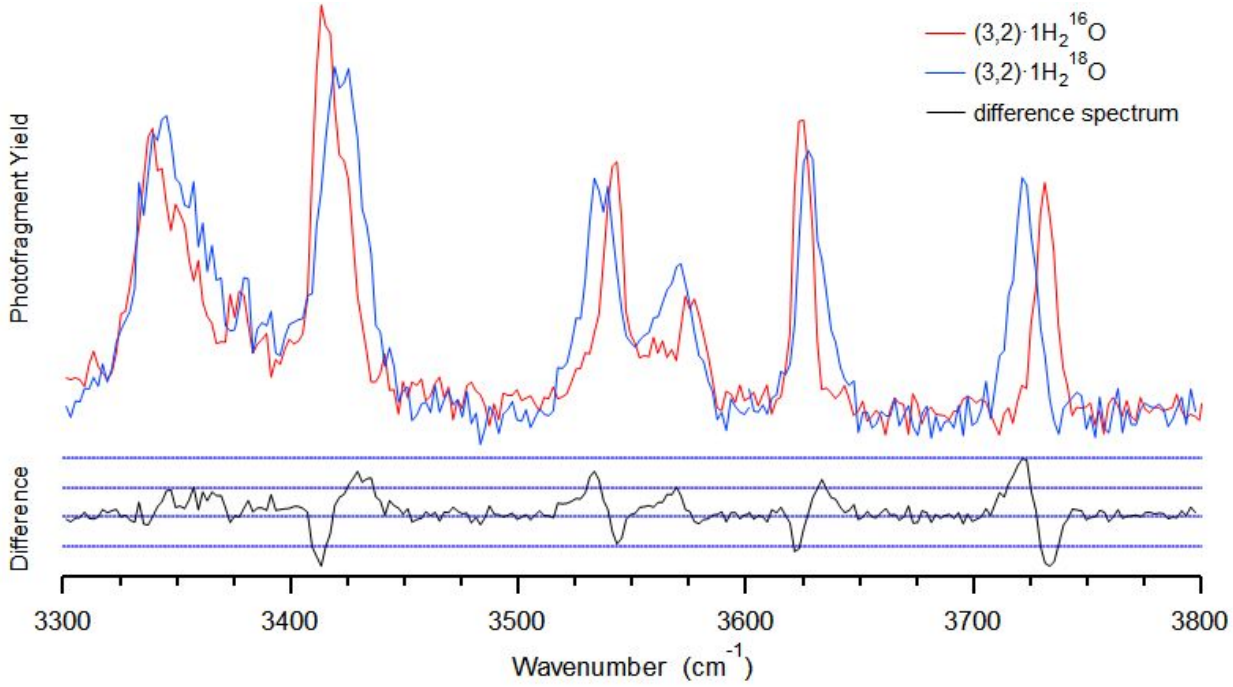


Figure S3. CIVP and difference spectra between singly N_2 tagged (3,2) with $H_2{}^{16}O$ and $H_2{}^{18}O$.

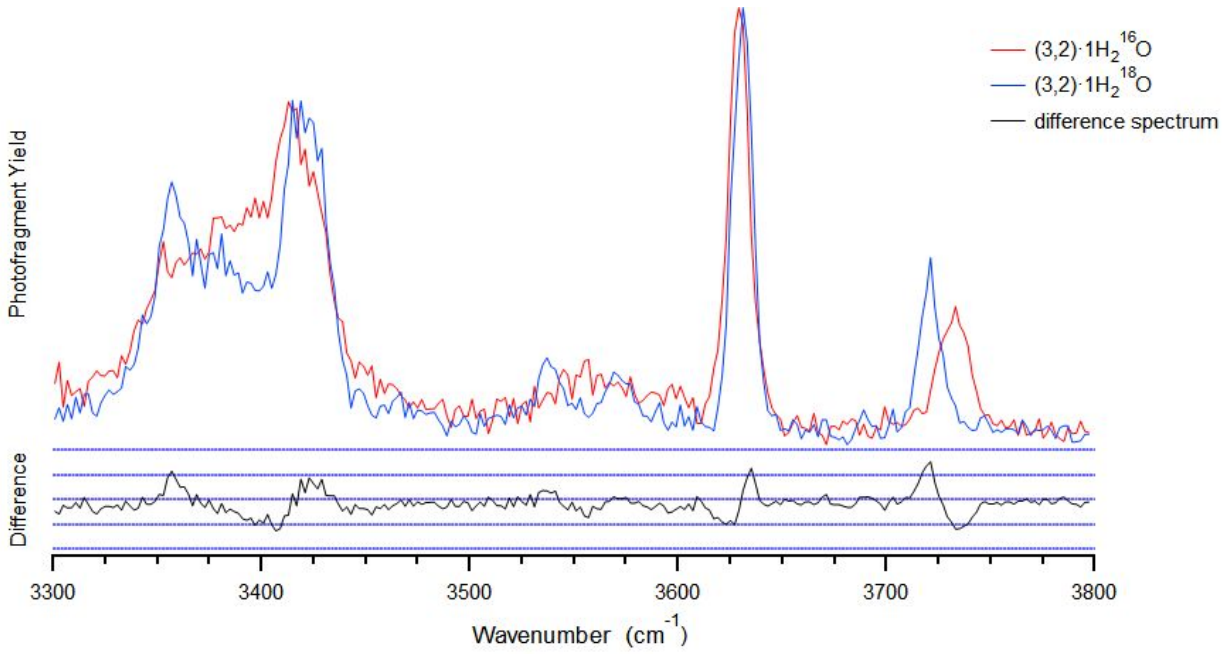


Figure S4. IRMPD and difference spectra between (3,2) cluster with $H_2{}^{16}O$ and $H_2{}^{18}O$.

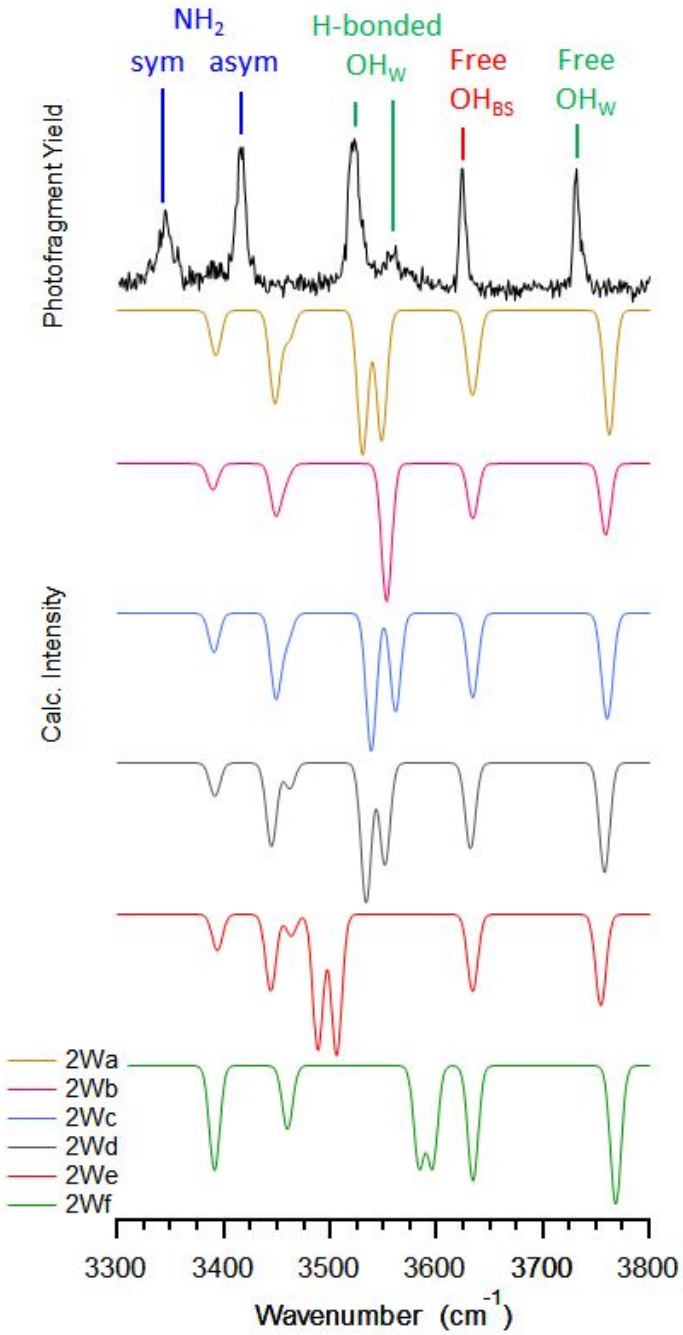


Figure S5. Comparison between N_2 tagged and calculated spectra of six isomers of $(3,2)\cdot 2H_2O$.

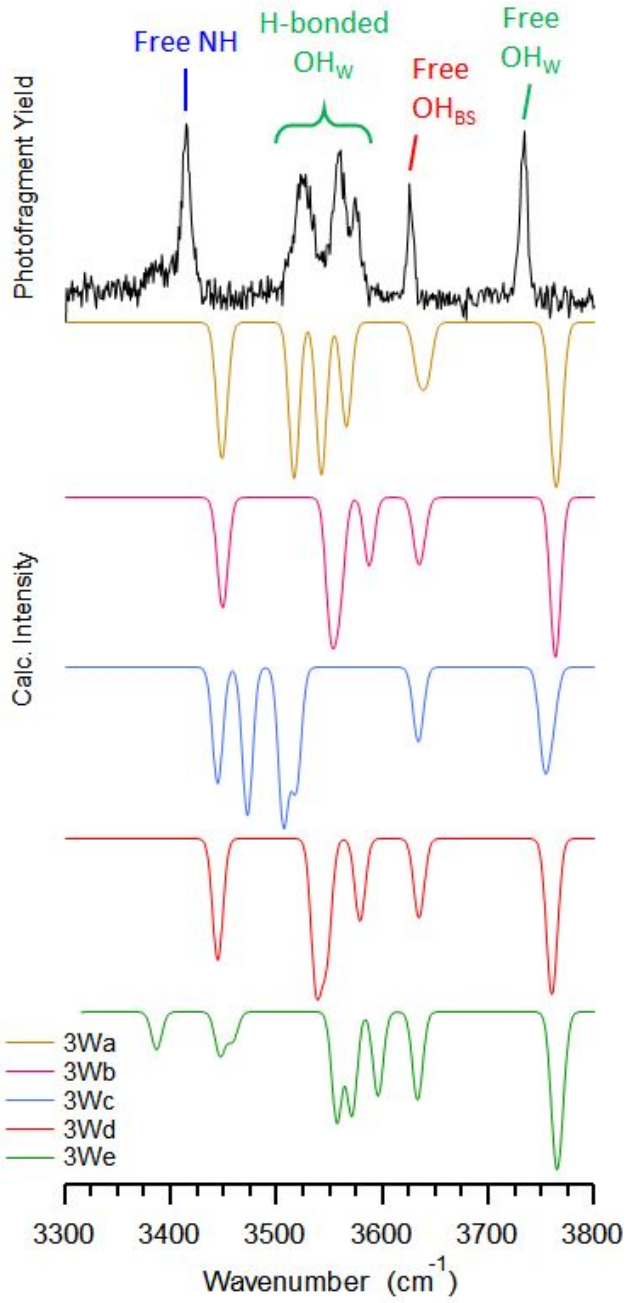


Figure S6. Comparison between N_2 tagged and calculated spectra of five isomers of $(3,2)\cdot 3H_2O$.

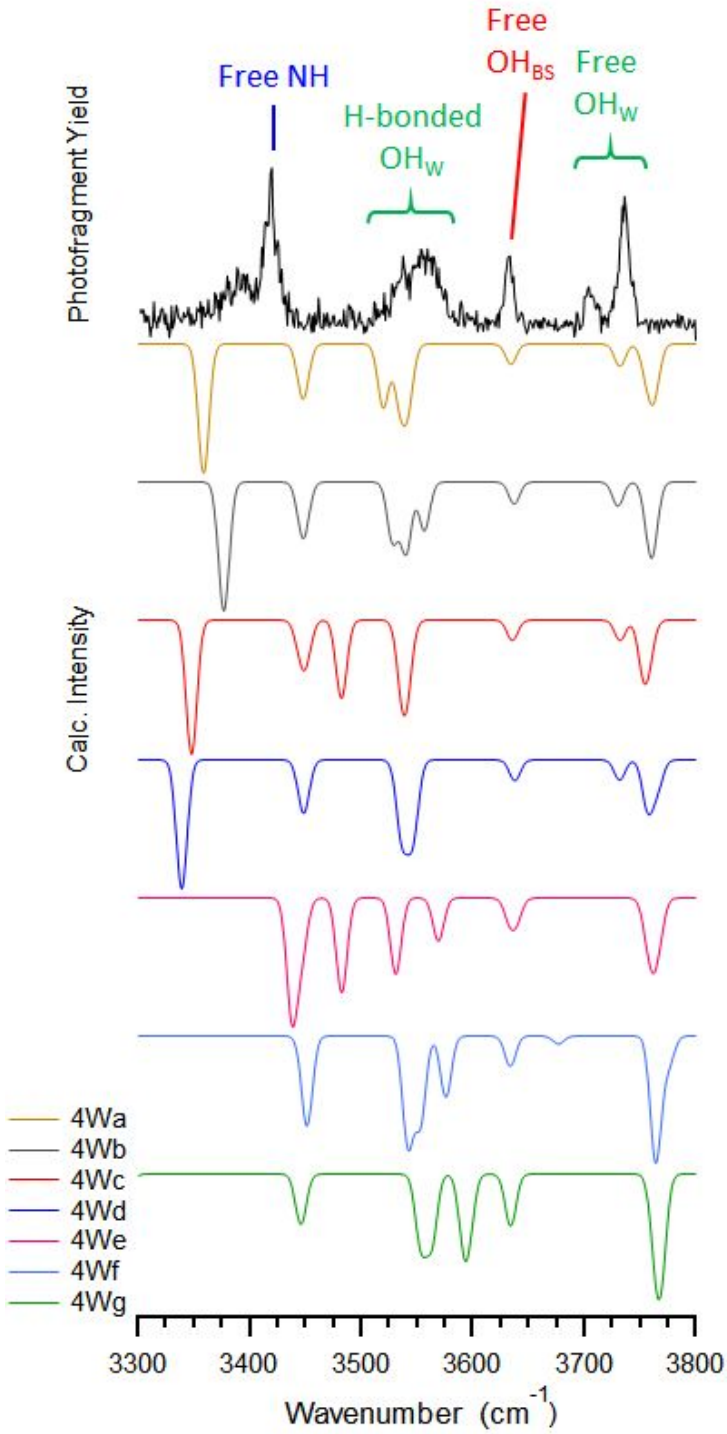
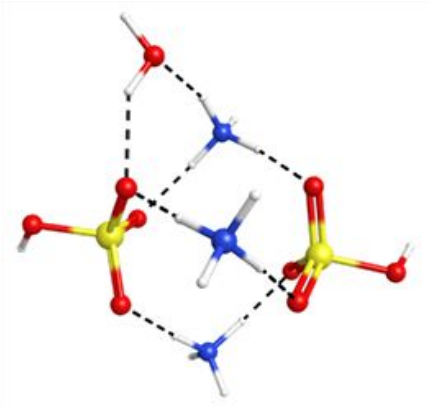


Figure S7. Comparison between N_2 tagged and calculated spectra of seven isomers of $(3,2)\cdot 4H_2O$.

Coordinates of the calculated structures

1. 1Wa



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1 0.306835 1.245605 3.153638
1 -0.741811 0.367743 2.148165
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7 0.852234 -2.837085 -0.883639
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1 1.416623 -3.434906 -0.278810
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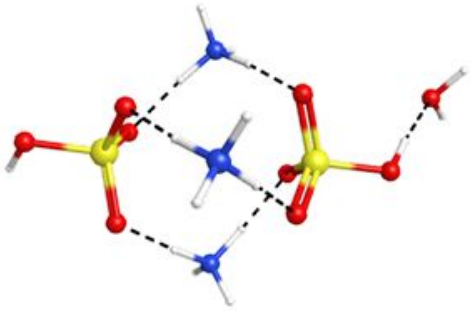
2. 1Wb



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1 0.250645 3.160351 -1.290256
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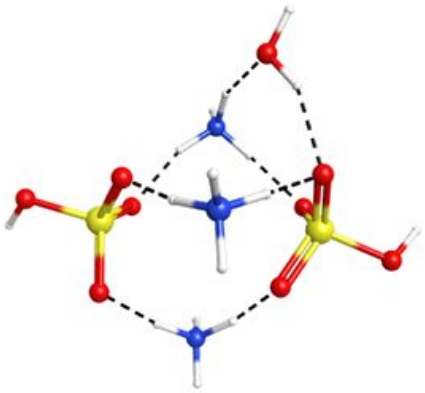
3. 1Wc



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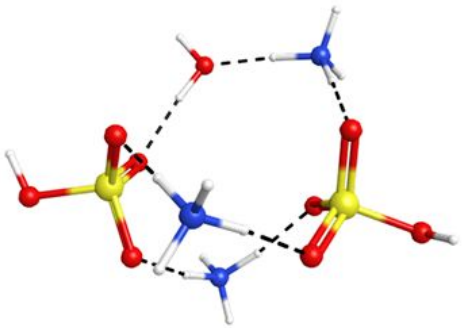
4. 1Wd



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1 1.226984 3.996143 -0.343114

5. 2Wa

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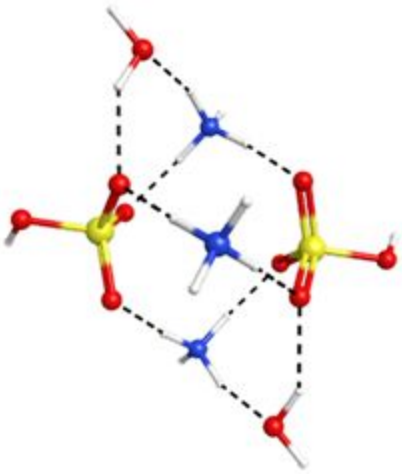
6. 2Wb



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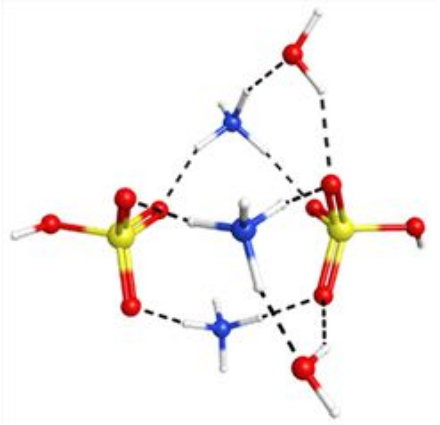
8. 2Wd



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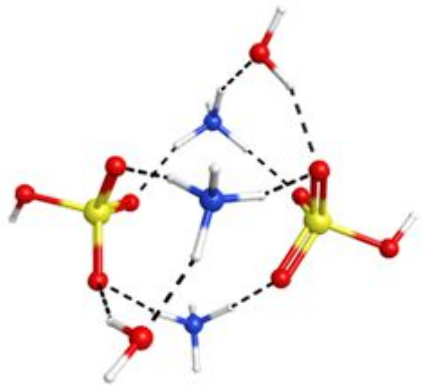
9. 2We



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7 -0.618288 -1.819614 -2.270688
1 0.256481 -1.705599 -1.686852
1 -1.429820 -1.561155 -1.654098
1 -0.590871 -1.187255 -3.071001
1 -0.701993 -2.782395 -2.597234
16 2.363546 -0.450061 -0.292255
8 3.785916 -1.248043 -0.473670
1 4.508890 -0.598008 -0.504479
8 2.334096 0.630621 -1.336321
8 1.357081 -1.550611 -0.484492
8 2.327216 0.086576 1.125005
16 -2.338403 0.477227 -0.190762
8 -1.720487 0.841533 1.118629
8 -1.686623 1.125720 -1.387617
8 -2.501220 -1.019815 -0.423070
8 -3.852391 1.091781 -0.047064
1 -4.345063 0.916178 -0.867156
8 1.563528 2.735951 1.634350
1 2.050053 1.890805 1.568759
1 2.089739 3.328088 2.183844
8 -1.584171 -2.851106 1.524876

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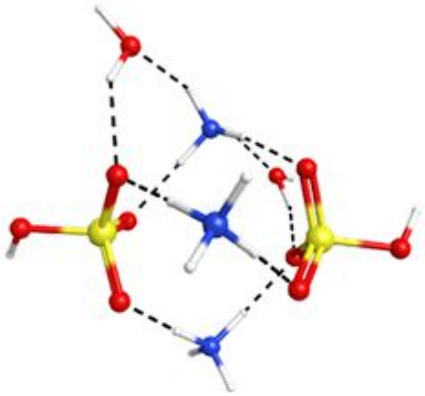
1 -2.153515 -3.524982 1.914197

10. 2Wf



7 -0.075565 2.503948 -0.024302
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1 -0.634175 1.878469 -0.632972
1 -0.737996 3.016314 0.578632
7 -0.463195 -1.778367 2.387268
1 0.389301 -1.823839 1.768256
1 -0.202252 -1.424378 3.308166
1 -1.155174 -1.129806 1.930703
1 -0.875944 -2.706612 2.483791
7 0.578246 -1.867220 -2.279691
1 1.228133 -1.138075 -1.892226
1 -0.303180 -1.877276 -1.699412
1 0.352242 -1.660389 -3.252791
1 1.034856 -2.778263 -2.221201
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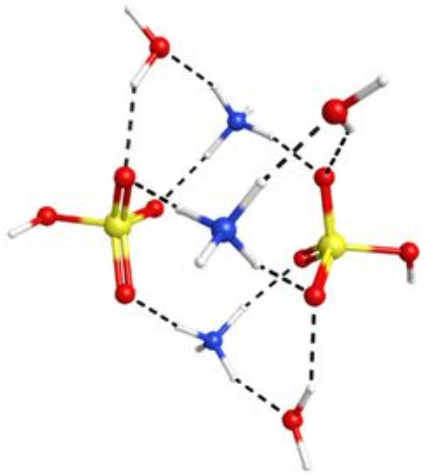
8 3.790423 -0.615409 0.856180
1 4.173971 0.248316 1.086671
8 1.661128 0.663314 1.333188
8 2.208845 0.005132 -1.038729
8 1.623704 -1.764206 0.618405
16 -2.200785 -0.463663 -0.444710
8 -2.107359 -0.057175 1.009539
8 -1.637996 0.541971 -1.407802
8 -1.659864 -1.854600 -0.685267

8 -3.826926 -0.515061 -0.664899
1 -4.014450 -0.618399 -1.613723
8 -2.212304 2.788050 1.716819
1 -2.519885 1.873176 1.604997
1 -2.950392 3.288202 2.083024
8 2.088542 2.850749 -1.718555
1 2.720950 3.309870 -2.282176
1 2.385394 1.927530 -1.650726

11. 3Wa



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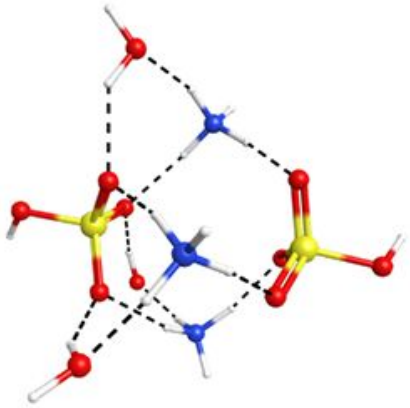
1 -0.765622 -0.353403 1.983172
1 -0.188331 -1.862179 2.406756
7 1.065347 -1.617473 -2.181334
1 1.333531 -0.622601 -2.020981
1 1.805519 -2.194384 -1.720940
1 0.152846 -1.773504 -1.710915
1 0.997594 -1.822264 -3.176742
7 -0.791433 2.953203 -0.677463
1 0.057485 2.727758 -0.112503
1 -1.073174 2.093797 -1.189123
1 -1.580472 3.193214 -0.042597
1 -0.595996 3.711344 -1.329222
16 2.180812 1.046875 0.152196
8 3.702278 1.667254 0.090915

1 3.962819 1.942039 0.986860
8 2.284250 -0.275387 0.895337
8 1.319187 2.029429 0.900836
8 1.829547 0.905204 -1.296755
16 -2.082133 -0.505705 -0.522925
8 -1.240474 -1.756663 -0.533333
8 -2.109131 0.142031 0.846677
8 -1.767569 0.458334 -1.630846
8 -3.600026 -1.073109 -0.807492
1 -4.089010 -0.397181 -1.306618
8 -0.736087 -3.369264 1.741914
1 -1.140127 -3.117506 0.892845
1 -1.166958 -4.177885 2.040844
8 2.978012 -2.627387 -0.510400
1 3.018924 -1.853647 0.083091
1 3.850701 -3.036485 -0.512051
8 -2.990262 2.832987 0.960432
1 -2.940923 1.874994 1.131416
1 -3.586171 3.219713 1.611208

12. 3Wb



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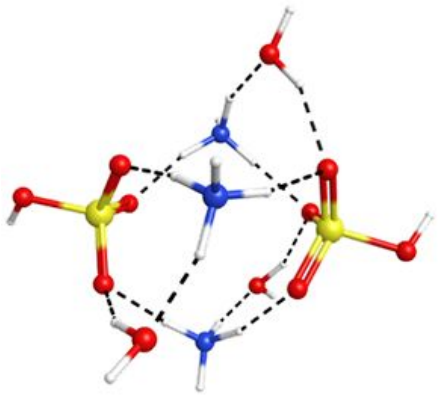
1 0.238118 2.784816 1.788291
7 -0.312648 0.954242 -2.754614
1 -1.101717 0.466092 -2.261622
1 -0.662234 1.712891 -3.337405

1 0.328949 1.311417 -2.027352
1 0.225963 0.258728 -3.314396
7 -0.462362 -2.818432 0.502113
1 -1.235702 -2.149716 0.745517
1 0.185602 -2.340157 -0.145994
1 0.084579 -3.041910 1.359374
1 -0.840999 -3.660162 0.070800
16 -2.615770 0.020212 0.019921
8 -4.240432 -0.074242 -0.209144
1 -4.688140 0.299932 0.568821
8 -2.294976 1.471095 0.284951
8 -2.266628 -0.865516 1.192496
8 -2.082085 -0.503528 -1.284094
16 1.983678 -0.015616 0.042091
8 1.544650 1.285048 -0.567799
8 1.576919 -0.160804 1.490936
8 1.628904 -1.234132 -0.775056
8 3.622441 0.127523 0.004188
1 4.021105 -0.690587 0.347658
8 1.346654 3.749110 0.834133
1 1.773350 3.103299 0.245919
1 1.963060 4.479535 0.959489
8 1.312871 -1.090091 -3.603897
1 1.934983 -1.374858 -4.282717
1 1.707211 -1.297075 -2.738157
8 1.364126 -2.799040 2.560053
1 1.604213 -1.860977 2.455338
1 1.531605 -3.042027 3.477616

13. 3Wc



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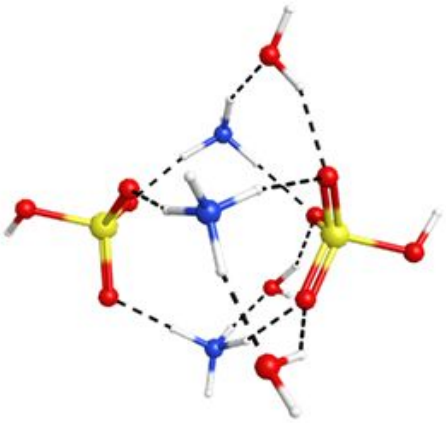
1 0.497163 -2.351458 2.983415
1 -0.522855 -1.506543 1.927052
1 0.552937 -2.726053 1.331231
7 -0.348479 -0.655346 -2.750514
1 0.619364 -0.674657 -2.384052
1 -0.420604 -1.228168 -3.590232
1 -0.981833 -1.018258 -2.002375
1 -0.674484 0.317728 -2.941363
7 -0.292275 2.735589 0.778552
1 0.395706 2.386088 0.079446
1 -1.173450 2.197651 0.635938
1 0.132090 2.551638 1.712583
1 -0.460569 3.732214 0.649295
16 2.333170 0.217710 -0.406449
8 3.852244 0.733895 -0.754135
1 4.486208 0.031888 -0.527482
8 2.303962 -0.054831 1.084424
8 1.489603 1.369334 -0.850965
8 2.084328 -1.032821 -1.220006
16 -2.472979 -0.283195 0.387951
8 -1.974612 -1.273284 -0.617195
8 -1.845810 -0.414525 1.751075
8 -2.443298 1.159982 -0.089341
8 -4.056020 -0.695014 0.529992
1 -4.455302 -0.161528 1.238573
8 1.223327 -3.479074 -0.116191
1 1.717988 -2.784394 -0.590360
1 1.632736 -4.325058 -0.329490
8 -1.674559 1.770196 -2.711007
1 -2.176903 1.618443 -1.885344
1 -2.266603 2.223478 -3.322444
8 1.302835 1.879832 2.873695
1 1.833788 2.293034 3.564424
1 1.897299 1.297088 2.363496

14. 3Wd



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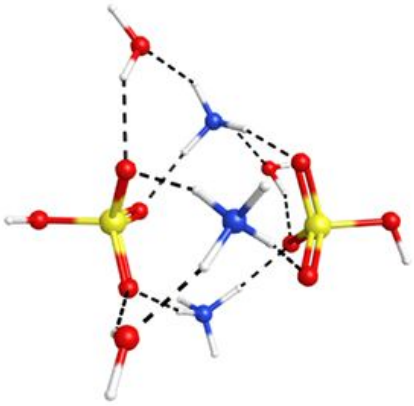
1 -0.698692 -3.631034 -1.120285
1 -1.386714 -2.131806 -0.716233
1 -0.311057 -2.290508 -2.073923
7 0.102862 2.392759 -1.687071
1 0.845861 1.685150 -1.816135
1 -0.072189 2.890951 -2.558587
1 -0.758790 1.869837 -1.391461
1 0.429617 3.048216 -0.945522
7 -0.300828 0.318832 2.876686
1 0.479895 0.674750 2.298458
1 -1.190162 0.450697 2.325804
1 -0.097113 -0.687099 3.052181
1 -0.354739 0.831001 3.755990
16 2.220898 -0.144025 -0.014776
8 3.841339 -0.116171 0.259228
1 4.277709 -0.735376 -0.350940
8 1.743278 -1.538311 0.314732
8 1.730656 0.909004 0.939085
8 2.009919 0.211368 -1.466509
16 -2.663962 0.133683 0.015956
8 -1.857873 0.631576 -1.149681
8 -2.558862 -1.360980 0.191492
8 -2.442406 0.883716 1.305258
8 -4.202011 0.470794 -0.454548
1 -4.804077 0.247205 0.275816
8 0.663106 -1.471522 -3.327800
1 1.326504 -0.923707 -2.871059
1 1.012159 -1.682122 -4.201071
8 1.289224 3.658322 0.468389
1 1.821315 4.437504 0.667087

1 1.780973 2.881248 0.785145
8 0.697636 -2.266937 2.839503
1 1.092107 -2.903543 3.446634
1 1.302753 -2.176210 2.080837

15. 3We



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1 0.571961 -0.909461 2.200274
1 -0.139758 0.148618 3.273362
7 -0.971030 2.523977 -0.602688
1 -1.291638 1.634837 -1.030935
1 -1.788746 2.959046 -0.151666
1 -0.275126 2.272105 0.120208
1 -0.487574 3.093922 -1.310212
7 0.950118 -1.984522 -1.871522
1 0.070536 -2.131499 -1.326500
1 1.255278 -1.003789 -1.733642
1 1.703027 -2.591297 -1.482447
1 0.791202 -2.173356 -2.860087
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8 -3.630823 -1.534714 -0.801667
1 -3.914164 -2.256682 -0.214634
8 -2.375617 -0.317585 1.034054
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8 0.981838 1.435776 1.190005

8 2.002512 -0.839801 1.131854
8 2.005627 0.550914 -0.960993
8 3.426342 1.271735 1.005241
1 4.159300 0.864137 0.512418
8 -3.190039 2.486003 1.064096
1 -4.077591 2.798891 1.272811
1 -3.217854 1.514620 1.112453
8 1.136316 3.028499 -2.330316
1 1.697837 3.585775 -2.880639
1 1.691192 2.296566 -2.013643
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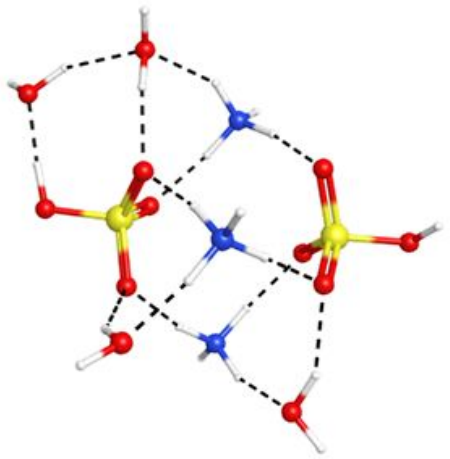
1 3.482625 -3.790544 -0.073335

16. 4Wa



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1 -0.451835 2.048723 2.317088
7 -1.406937 1.419284 -2.241961
1 -1.566426 0.407902 -2.053739
1 -2.239771 1.920455 -1.860896
1 -0.551581 1.704648 -1.722124
1 -1.293071 1.589376 -3.239657
7 0.819458 -2.759144 -0.562311
1 -0.040461 -2.625786 0.019137
1 1.015523 -1.853462 -1.052914

1 1.632983 -2.948036 0.045056
1 0.678587 -3.512490 -1.233660
16 -2.361367 -1.266710 0.155980
8 -3.777571 -2.099462 0.080772
1 -4.050852 -2.331422 0.984935
8 -2.677520 0.059453 0.826777
8 -1.398714 -2.083972 0.980040
8 -1.978367 -1.148409 -1.286397
16 1.708428 0.753671 -0.430784
8 0.767731 1.930664 -0.519182
8 1.666573 0.097934 0.950839
8 1.480203 -0.256789 -1.525415
8 3.164493 1.403156 -0.615264
1 3.866699 0.680619 -0.559967
8 0.001420 3.568836 1.622003
1 0.478859 3.303800 0.814562
1 0.363985 4.413700 1.910875
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8 3.126480 -2.235191 1.068543
1 2.672254 -1.377042 1.232697
1 3.434479 -2.557283 1.925109
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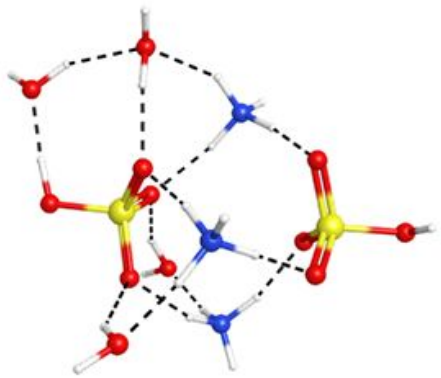
1 5.563456 -0.800832 -1.015269
1 4.544140 -1.333965 0.047367

17. 4Wb



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1 0.488107 2.284572 -2.460158
7 1.095307 1.690887 2.298591
1 1.689461 0.905529 1.937439
1 1.672350 2.481663 2.579613
1 0.440674 1.959089 1.542144
1 0.510174 1.344521 3.090022
7 0.013079 -2.714827 0.414329
1 0.864333 -2.382979 -0.111854
1 -0.419151 -1.889364 0.878595
1 -0.689117 -3.084033 -0.245873
1 0.276818 -3.417873 1.103192
16 2.812769 -0.585402 -0.156877
8 4.367403 -1.079728 0.047772
1 4.820137 -1.046122 -0.812174
8 2.872108 0.749928 -0.855486
8 2.105522 -1.636588 -0.982015
8 2.308294 -0.529824 1.257723
16 -1.629853 0.542368 0.097794
8 -0.936012 1.865965 0.274716
8 -1.283518 -0.121950 -1.228966
8 -1.390304 -0.410845 1.252640
8 -3.192195 0.912875 0.071827
1 -3.730670 0.074622 -0.090907
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1 -0.802908 3.315602 -1.023437
1 -0.776053 4.461623 -2.085489
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1 -1.391135 0.604441 4.600794
1 -1.297658 0.112646 3.120090
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1 -1.908145 -1.785579 -1.585019
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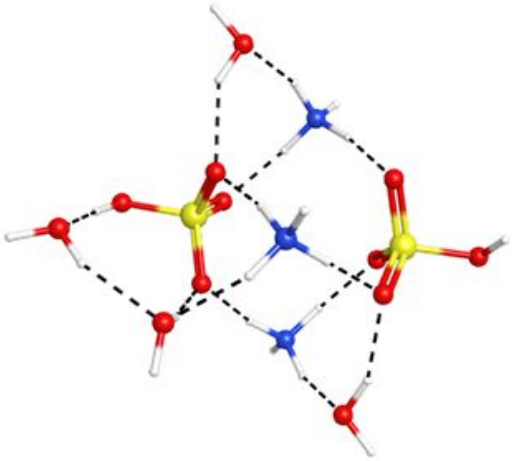
8 -4.488133 -1.318311 -0.456781
1 -3.901877 -2.052523 -0.718181
1 -5.217710 -1.690356 0.052215

18. 4Wc



7 0.190992 -0.673224 -2.363910
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1 0.709671 0.015068 -1.765732
1 0.730289 -1.554566 -2.321374
7 -1.046677 -1.681653 2.286672
1 -1.609854 -0.842725 2.031149
1 -1.503125 -2.491134 1.812828
1 -0.094401 -1.548679 1.887012
1 -1.005722 -1.804951 3.296666
7 -0.427890 3.105621 0.702593
1 -1.111802 2.623500 0.081391
1 0.041429 2.385091 1.288060
1 0.314476 3.550273 0.117987
1 -0.901385 3.792410 1.287120
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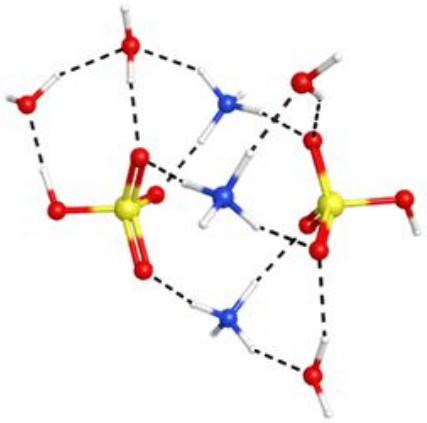
8 -4.288674 0.513328 -0.550879
1 -4.469953 0.722376 -1.483223
8 -2.252923 -0.929144 -1.012411
8 -2.022136 1.557163 -1.032796
8 -2.520871 0.371927 1.140883
16 1.753084 0.223373 0.800674
8 1.266070 -1.224532 0.768438
8 1.632088 0.850379 -0.582548
8 1.090029 1.018762 1.877213
8 3.316238 0.203150 1.174701
1 3.808416 -0.315089 0.465350
8 2.045482 -2.658138 -1.422333
1 1.775976 -2.330127 -0.533199

1 2.001177 -3.622076 -1.389532
8 -2.249662 -3.333714 0.445056
1 -2.474742 -2.601790 -0.163224
1 -2.977979 -3.964560 0.407124
8 1.699025 3.647599 -0.951872
1 2.029432 2.731210 -0.917368
1 2.467073 4.227239 -1.012017
8 4.445772 -1.180633 -0.791514
1 5.322150 -1.580967 -0.747727
1 3.842256 -1.846155 -1.170007

19. 4Wd



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1 0.642740 1.760435 2.531555
7 -0.904836 1.470822 -2.077874
1 -1.132776 0.468767 -1.840949
1 -1.677587 2.041347 -1.693348
1 -0.008185 1.707537 -1.606571
1 -0.820545 1.598971 -3.085056
7 1.134745 -2.915323 -0.703005
1 0.329902 -2.690090 -0.071193
1 1.359770 -2.057596 -1.240986
1 1.975997 -3.139239 -0.133802
1 0.895022 -3.681717 -1.329603
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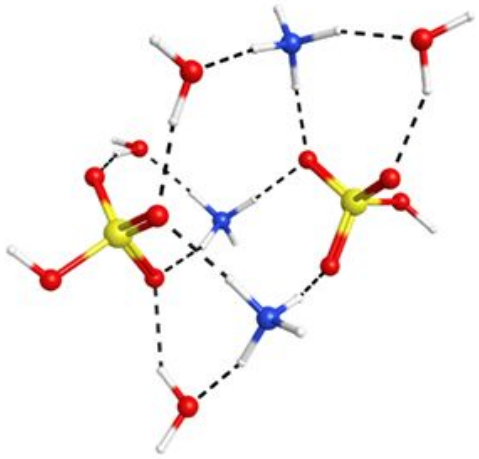
20. 4We



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8 2.378426 -0.724170 0.493517
8 1.569972 0.534437 -1.516744
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1 2.107220 2.178209 2.152014
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1 0.518998 2.010079 -1.757801
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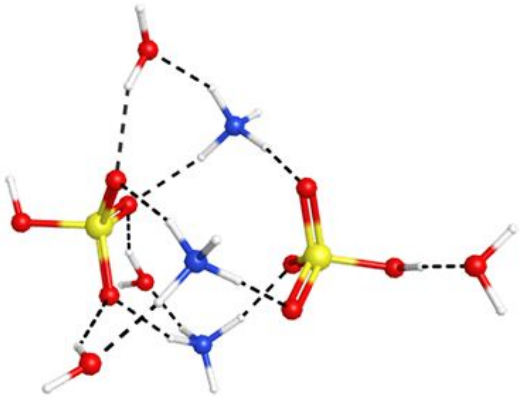
21. 4Wf



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1 -0.043463 3.218605 0.128976
7 0.354015 -0.669136 -2.854364
1 -0.432833 -1.008508 -2.238911
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1 0.816108 0.112736 -2.362396
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7 0.083880 -2.255011 1.773784
1 -0.764426 -1.661343 1.570418
1 0.786775 -2.071923 1.039246
1 0.507783 -1.957616 2.675222
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8 -1.941267 -0.519153 1.205219
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16 2.299611 0.304427 0.190155
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8 1.676957 0.814737 1.469394
8 2.221738 -1.198796 0.077400
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1 4.318180 0.236343 0.976532
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1 3.125059 -2.953015 -2.827312
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8 1.565958 -0.949409 3.701124
1 1.722714 -0.165480 3.143981
1 1.615973 -0.666359 4.620953
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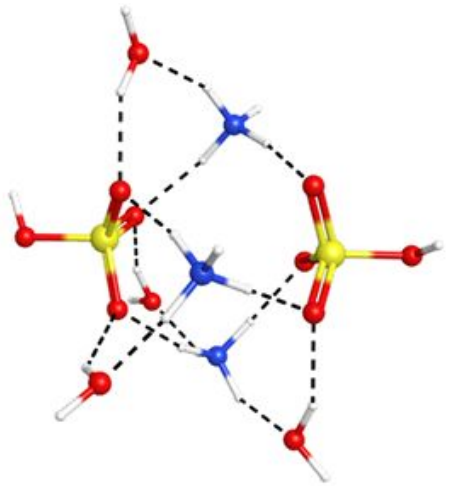
22. 4Wg



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1 -0.141967 -2.012655 0.933006
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1 1.364553 3.235207 0.563752
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8 1.896425 0.173573 1.351371
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1 4.232909 -0.319322 0.190028
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1 1.131280 -2.685315 -2.010953
1 1.039938 -3.414131 -3.391021
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1 1.660013 -1.864889 4.317890
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