

## **Supporting Information I**

(xyz coordinates, Å)

### **Structure and Solvation Dynamics of the Hydroxide Ion in Ice-like Water Clusters: a CCSD(T) and Car-Parrinello Molecular Dynamics Study**

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## MP2/aVDZ optimized geometries

OH(H<sub>2</sub>O)<sub>8</sub>

## 8w-I

8	-1.100999000	-2.138004000	0.721406000
8	0.760396000	-2.725423000	-1.287536000
8	1.442893000	-4.375298000	0.561307000
8	-1.449796000	-3.557649000	-2.322776000
8	-1.221187000	-5.266364000	-0.029620000
8	2.425544000	-6.589451000	-0.997863000
8	2.060157000	-4.550964000	-2.995535000
8	-0.309611000	-5.687655000	-3.926734000
8	-0.202962000	-7.439420000	-1.688840000
1	-0.420127000	-2.253933000	0.014439000
1	1.415703000	-3.903706000	1.403053000
1	1.287470000	-3.650333000	-0.140048000
1	-0.578476000	-3.131363000	-2.011319000
1	1.238726000	-1.921374000	-1.530183000
1	-1.372805000	-4.728351000	-0.835418000
1	-0.306506000	-5.026530000	0.228722000
1	2.331535000	-5.255257000	-2.370371000
1	0.576506000	-5.301034000	-3.731200000
1	-0.668068000	-6.857546000	-1.056355000
1	2.206840000	-5.940526000	-0.304224000
1	1.555418000	-6.996263000	-1.205538000
1	1.641502000	-3.877981000	-2.406393000
1	-0.284347000	-6.936321000	-2.529436000
1	-0.900958000	-4.997817000	-3.576071000
1	-2.119710000	-2.891231000	-2.124904000
1	-1.446736000	-3.038459000	0.815798000

## 8w-II

8	-1.161487000	-2.605437000	0.748111000
8	0.750546000	-2.566138000	-1.298123000
8	1.776969000	-4.253384000	0.346363000
8	0.986967000	-0.211008000	-0.274626000
8	3.405475000	-2.264771000	-2.194021000
8	4.591584000	-3.806649000	-0.074852000
8	4.563765000	-1.382378000	1.417729000
8	1.736176000	-1.869278000	1.943810000
8	3.805688000	0.148234000	-0.855729000
1	-0.556428000	-2.614615000	-0.033348000
1	0.092493000	0.111510000	-0.107361000
1	0.843766000	-1.077628000	-0.790669000
1	1.341784000	-3.693135000	-0.387495000
1	0.329055000	-2.784654000	-2.140004000
1	1.786965000	-2.723188000	1.465062000
1	1.499677000	-1.231979000	1.236940000
1	3.667663000	-1.501137000	1.789037000
1	2.867838000	0.309534000	-0.648540000
1	2.464125000	-2.392062000	-1.924101000
1	3.710095000	-4.149832000	0.160284000
1	1.069224000	-4.830930000	0.658140000
1	-0.554196000	-2.379471000	1.468795000
1	3.742130000	-0.648137000	-1.434276000
1	3.893162000	-2.858832000	-1.585870000
1	4.682289000	-3.012887000	0.497462000
1	4.395934000	-0.770435000	0.666900000

## 8w-III

8	-0.730718000	-2.192793000	0.926827000
8	0.786798000	-2.721523000	-1.349864000
8	1.448644000	-4.335166000	0.572387000
8	-1.522595000	-3.672060000	-2.318247000
8	-1.213993000	-5.338177000	-0.096644000
8	2.396271000	-6.542885000	-0.960951000
8	1.932013000	-4.555211000	-2.953911000
8	-0.188518000	-5.693666000	-4.010370000
8	-0.216197000	-7.457952000	-1.683986000
1	-0.235315000	-2.287673000	0.074129000
1	1.153369000	-3.851679000	1.356846000
1	1.311734000	-3.651177000	-0.166155000
1	-0.684469000	-3.190762000	-2.070694000
1	1.236478000	-1.888280000	-1.545869000
1	-1.420010000	-4.753231000	-0.864231000
1	-0.319332000	-5.044063000	0.169995000
1	2.244198000	-5.226718000	-2.309442000
1	0.657974000	-5.260240000	-3.677031000
1	-0.674323000	-6.821987000	-1.090626000

1	2.167270000	-5.912581000	-0.251939000
1	1.538316000	-6.974998000	-1.162946000
1	1.548271000	-3.830135000	-2.376803000
1	-0.277898000	-7.018717000	-2.552396000
1	-0.052170000	-5.813927000	-4.957021000
1	-1.237846000	-4.275984000	-3.025981000
1	-1.385874000	-2.902355000	0.862376000

## 8w-IV

8	-1.054405000	-2.991487000	0.654612000
8	0.805075000	-2.517150000	-1.366323000
8	1.728443000	-4.260645000	0.320232000
8	1.080789000	-0.141160000	-0.161025000
8	3.384782000	-2.189083000	-2.062579000
8	3.923960000	0.116588000	-0.921476000
8	1.802764000	-1.831147000	1.943485000
8	4.562924000	-1.396280000	1.492455000
8	4.523987000	-3.823798000	-0.021157000
1	-0.473674000	-2.764333000	-0.115220000
1	0.902871000	-0.937000000	-0.320232000
1	1.364032000	-3.678424000	-0.428251000
1	0.341387000	-2.738398000	-2.185453000
1	1.799083000	-2.674650000	1.447000000
1	1.507371000	-1.175123000	1.268078000
1	3.631766000	-1.492005000	1.792689000
1	2.412047000	-2.330015000	-1.862660000
1	3.642862000	-4.164642000	0.223522000
1	0.919564000	-4.600576000	0.728215000
1	-0.679025000	-2.446830000	1.361230000
1	3.758771000	-0.742480000	-1.421698000
1	3.839599000	-2.834648000	-1.479380000
1	4.635440000	-3.046271000	0.567599000
1	4.481776000	-0.771497000	0.748126000
1	1.960220000	0.157315000	-0.451168000
1	4.424409000	0.669656000	-1.532098000

## 8w-V

8	-2.087905000	-0.004021000	-0.009599000
1	-1.504416000	-1.111064000	-1.101590000
8	-1.077725000	-1.768217000	-1.728830000
1	-1.009195000	-1.269755000	-2.554100000
1	0.759399000	-1.829835000	-1.210143000
8	1.715908000	-1.702239000	-1.045778000
1	1.773092000	-1.563784000	-0.074317000
1	-1.518997000	1.105640000	1.087331000
1	-1.514783000	-1.097906000	1.101267000
1	-1.508231000	1.092593000	-1.114540000
8	-1.100263000	1.764546000	1.718060000
8	-1.093802000	-1.726692000	1.760552000
8	-1.083405000	1.723535000	-1.769269000
1	-1.037323000	1.266677000	2.544134000
1	-1.023739000	-2.551541000	1.261589000
1	-1.020156000	2.547869000	-1.268533000
1	0.741486000	1.832358000	1.216531000
1	0.744270000	-1.212538000	1.834539000
1	0.756870000	1.215123000	-1.827456000
8	1.699939000	1.708107000	1.061206000
8	1.702010000	-1.050734000	1.713069000
8	1.714056000	1.056525000	-1.697653000
1	1.766779000	1.569837000	0.090336000
1	1.762697000	-0.079440000	1.574963000
1	1.776842000	0.085441000	-1.558961000
1	-3.055105000	-0.006147000	-0.015117000

OH(H<sub>2</sub>O)<sub>9</sub>

## 9w-I

8	-0.664670000	-1.906441000	0.791847000
8	0.589966000	-2.816735000	-1.393356000
8	1.016661000	-5.075501000	-0.096330000
8	2.244855000	-1.151919000	-0.098970000
8	2.720347000	-3.432059000	1.486648000
8	4.610868000	-1.876739000	-1.677045000
8	2.825229000	-3.473048000	-2.757383000
8	3.489221000	-5.831220000	-1.330477000
8	5.162513000	-4.053546000	0.198566000
1	-0.260752000	-2.258597000	-0.057256000
1	3.084443000	-1.133039000	-0.591217000
1	1.633314000	-1.658290000	-0.702526000

1	0.739763000	-4.285410000	-0.653507000
1	-0.044806000	-2.670708000	-2.108230000
1	2.224570000	-4.046992000	0.902374000
1	2.562592000	-2.564138000	1.047295000
1	3.048180000	-4.362115000	-2.404076000
1	4.132355000	-5.341126000	-0.775871000
1	4.416792000	-3.821145000	0.793270000
1	5.126878000	-1.458233000	-2.375750000
1	3.955320000	-2.472536000	-2.158458000
1	1.968877000	-3.241977000	-2.293620000
1	5.174303000	-3.300912000	-0.421212000
1	2.658042000	-5.779760000	-0.819916000
1	0.434702000	-5.034690000	0.685054000
1	-0.039445000	-1.208205000	1.034114000
8	-0.089140000	-4.100395000	2.449706000
1	0.853910000	-3.891541000	2.560849000
1	-0.400738000	-3.315696000	1.944098000

**9w-II**

8	-0.621197000	-1.924267000	0.857221000
8	0.530578000	-2.844053000	-1.358999000
8	1.038365000	-5.060750000	-0.096933000
8	2.250082000	-1.163508000	-0.140274000
8	2.759272000	-3.458015000	-2.860322000
8	4.611571000	-1.810063000	-1.630153000
8	-0.019841000	-4.106028000	2.490082000
8	2.781218000	-3.414039000	1.343855000
8	5.135272000	-4.056308000	0.267591000
8	3.455917000	-5.872846000	-1.365473000
1	-0.258260000	-2.275079000	-0.014318000
1	3.090322000	-1.184847000	-0.645039000
1	1.616910000	-1.656361000	-0.728384000
1	0.730660000	-4.270530000	-0.654060000
1	-0.116740000	-2.734475000	-2.068982000
1	2.217457000	-4.030892000	0.819513000
1	2.586857000	-2.539558000	0.916454000
1	3.000082000	-4.342867000	-2.523132000
1	4.306623000	-3.801501000	0.763760000
1	4.010780000	-2.374645000	-2.175292000
1	1.933286000	-3.239378000	-2.353621000
1	2.623936000	-5.778307000	-0.860581000
1	0.454395000	-5.051483000	0.682995000
1	0.008483000	-1.218496000	1.063858000
1	0.925170000	-3.909430000	2.592246000
1	-0.327462000	-3.316604000	1.985647000
1	5.008439000	-2.460445000	-1.025854000
1	4.109176000	-5.397554000	-0.821323000
1	5.774293000	-4.287908000	0.951579000

**9w-III**

8	-0.881524000	-1.490512000	0.512105000
8	0.725586000	-2.648574000	-1.216338000
8	1.418576000	-4.445958000	0.629617000
8	-1.494173000	-3.644997000	-2.112106000
8	-0.919940000	-3.720195000	2.264348000
8	-1.110539000	-5.575438000	-0.069182000
8	2.449369000	-6.597736000	-1.029958000
8	2.022179000	-4.511697000	-2.929487000
8	-0.327921000	-5.620184000	-3.937153000
8	-0.092052000	-7.586050000	-1.883828000
1	-0.224896000	-1.883723000	-0.154315000
1	0.907132000	-4.152618000	1.406489000
1	1.297503000	-3.704919000	-0.029421000
1	-0.624813000	-3.183350000	-1.856854000
1	1.233955000	-1.946310000	-1.645382000
1	-1.376154000	-4.948370000	-0.776769000
1	-0.181552000	-5.308175000	0.101771000
1	2.315203000	-5.232142000	-2.331480000
1	0.551486000	-5.233091000	-3.715673000
1	-0.584355000	-7.079542000	-1.208775000
1	2.177735000	-6.010119000	-0.301068000
1	1.615945000	-7.047727000	-1.290442000
1	1.591281000	-3.873630000	-2.315827000
1	-0.205572000	-7.019540000	-2.678291000
1	-0.930603000	-4.986315000	-3.509447000
1	-2.172471000	-2.983382000	-1.926765000
1	-1.284130000	-4.400667000	1.670377000
1	-0.996558000	-2.904399000	1.724378000
1	-0.402147000	-0.752248000	0.907856000

**9w-IV**

1	-0.020659000	-0.042941000	2.504260000
8	-0.091938000	-0.102022000	1.539790000
8	-2.219661000	-1.421001000	0.852760000
1	-1.400267000	-0.917260000	1.207980000
1	-2.682266000	-1.737757000	1.637230000
8	0.011970000	-0.009921000	-1.375230000
1	0.080749000	0.093160000	-0.405470000
1	-0.173267000	-0.975403000	-1.457250000
8	-1.444580000	2.235500000	0.873890000
1	-2.110605000	1.854871000	0.268730000
1	-0.979699000	1.425576000	1.205140000
8	2.224991000	1.407289000	0.968720000
1	1.436558000	0.885899000	1.251550000
1	1.823222000	2.085694000	0.389000000
8	-2.873288000	0.601060000	-1.058630000
1	-1.981926000	0.495873000	-1.440660000
1	-2.886888000	-0.133620000	-0.413750000
8	0.609021000	2.938348000	-0.873070000
1	-0.164088000	2.820857000	-0.271470000
1	0.518351000	2.179346000	-1.470320000
8	3.014357000	-0.517300000	-0.893350000
1	2.206886000	-0.401471000	-1.421410000
1	2.907108000	0.203189000	-0.229640000
8	-0.534353000	-2.733998000	-1.076990000
1	0.222908000	-2.771248000	-0.446450000
1	-1.275136000	-2.521108000	-0.478130000
8	1.474701000	-2.294231000	0.807580000
1	2.160155000	-1.837012000	0.279920000
1	0.949091000	-1.536448000	1.167020000

**9w-V**

8	-0.950691000	-1.615353000	0.577648000
8	0.659719000	-2.671295000	-1.214355000
8	0.937809000	-4.519689000	0.568104000
8	-1.463727000	-3.557737000	-2.587322000
8	-1.439153000	-5.574986000	-0.560975000
8	-3.182123000	-3.175245000	-0.223736000
8	2.312263000	-6.590677000	-0.934437000
8	2.111996000	-4.483957000	-2.859737000
8	-0.087307000	-5.624586000	-4.148018000
8	-0.071084000	-7.607863000	-2.104696000
1	-2.827592000	-4.072645000	-0.090483000
1	0.931869000	-3.747025000	-0.096703000
1	-0.660598000	-3.118367000	-2.190901000
1	1.330538000	-2.003486000	-1.413796000
1	-1.399553000	-5.005995000	-1.360479000
1	-0.648616000	-5.278817000	-0.060019000
1	2.332382000	-5.211768000	-2.240476000
1	0.750421000	-5.220608000	-3.822423000
1	-0.660220000	-7.114702000	-1.501241000
1	1.929451000	-6.005712000	-0.255449000
1	1.528658000	-7.052215000	-1.307748000
1	1.606802000	-3.856933000	-2.293211000
1	-0.094082000	-7.037975000	-2.905074000
1	-0.748226000	-4.988447000	-3.820934000
1	-2.200796000	-3.229685000	-2.039479000
1	-2.475009000	-2.608456000	0.152268000
1	-0.312846000	-1.963495000	-0.130280000
1	-1.087893000	-0.690979000	0.336367000
1	0.839211000	-4.094868000	1.429238000

**OH(H<sub>2</sub>O)<sub>10</sub>**

**10w-I**

8	0.069174000	0.800340000	0.683074000
8	-0.897187000	-1.715519000	0.644970000
8	0.426962000	-3.491663000	-1.239873000
1	-0.215091000	-0.153772000	0.717192000
1	0.681772000	-2.752238000	-1.818582000
1	-1.710722000	-1.599689000	-0.079412000
1	-0.363706000	-2.363915000	0.145156000
1	-0.444085000	-3.724058000	-1.616428000
1	-0.338533000	1.188328000	1.466795000
8	-3.067225000	-1.286508000	-0.945332000
8	-2.171110000	-3.275393000	-2.404037000
8	-1.509602000	0.725181000	-1.712453000
1	-0.952170000	0.966091000	-0.947594000

1	-2.161595000	0.065338000	-1.334786000
1	-2.628410000	-2.609133000	-1.801588000
1	-3.770839000	-1.311647000	-0.282015000
8	-0.276089000	-1.323963000	-3.201302000
1	-0.949078000	-2.005760000	-2.980804000
1	-0.585436000	-0.549346000	-2.678341000
8	-4.484278000	-0.644345000	-3.157950000
8	-1.600436000	-0.690350000	-5.627717000
8	-3.706173000	-2.564203000	-4.769677000
8	-2.828808000	1.431684000	-4.124135000
1	-4.036167000	0.164391000	-3.492070000
1	-4.078071000	-1.833071000	-4.182609000
1	-0.999745000	-0.918487000	-4.885443000
1	-2.287470000	1.395219000	-3.310547000
1	-2.367878000	0.814312000	-4.730509000
1	-3.997077000	-0.852840000	-2.309546000
1	-2.724216000	-3.304973000	-3.205174000
1	-4.472470000	-2.935216000	-5.222398000
1	-2.302848000	-1.360014000	-5.537707000

#### 10w-II

8	-2.897757000	-0.937032000	-1.102003000
8	-0.356480000	-0.451515000	-1.829336000
8	0.532707000	-2.256722000	-0.253949000
8	-0.659316000	1.614840000	-0.208182000
8	2.372842000	0.387129000	-1.879833000
8	3.291004000	-1.474001000	0.092316000
8	-0.162965000	-0.352358000	1.709147000
8	2.097368000	2.447147000	-0.005202000
8	2.618925000	0.518499000	2.008608000
8	-2.929843000	-0.876850000	1.819561000
1	-1.968269000	-0.707369000	1.934957000
1	-1.946067000	-0.803771000	-1.392315000
1	-1.614389000	1.803432000	-0.181670000
1	-0.562232000	0.941850000	-0.944993000
1	0.183993000	-1.625448000	-0.984720000
1	-0.369136000	-0.524250000	-2.793722000
1	0.083362000	-1.090569000	1.109476000
1	-0.311028000	0.396237000	1.083278000
1	2.807770000	-0.276447000	-1.303437000
1	3.155814000	-0.831652000	0.823807000
1	1.696613000	0.226259000	2.136336000
1	1.122616000	2.435713000	-0.001233000
1	2.291722000	1.817929000	-0.737795000
1	1.431736000	0.097686000	-1.879050000
1	2.511366000	1.270422000	1.383723000
1	2.429113000	-1.926397000	0.032567000
1	0.017373000	-3.066810000	-0.346710000
1	-3.283904000	-0.000381000	1.601428000
8	-3.558458000	1.454274000	-0.116038000
1	-4.222514000	1.926944000	-0.631073000
1	-3.401917000	0.599810000	-0.610019000
1	-2.836218000	-1.250498000	-0.179543000

#### 10w-III

8	-3.528931000	1.454061000	-0.236392000
8	-2.910954000	-1.028981000	-1.006325000
8	-0.334311000	-0.697473000	-1.767364000
8	0.517755000	-2.308128000	0.038395000
8	-0.636238000	1.534069000	-0.394944000
8	2.337682000	0.252704000	-1.898759000
8	3.287794000	-1.422775000	0.098810000
8	2.052005000	2.502654000	-0.151319000
8	-0.157108000	-0.182245000	1.751830000
8	-2.916533000	-0.657379000	1.842861000
8	2.638785000	0.647283000	1.940683000
1	-3.392911000	0.561385000	-0.665450000
1	-1.956915000	-0.472491000	1.953381000
1	-1.956734000	-0.949171000	-1.305289000
1	-2.840927000	-1.192980000	-0.045955000
1	-0.554208000	0.775775000	-1.047536000
1	0.189116000	-1.774736000	-0.772005000
1	-0.367221000	-0.888465000	-2.714989000
1	0.088424000	-0.986281000	1.240730000
1	-0.291618000	0.488945000	1.038412000
1	1.712711000	0.381383000	2.097039000
1	2.307399000	1.972221000	0.634924000
1	1.400383000	-0.052088000	-1.882014000
1	2.970701000	-0.085563000	1.375414000

1	-1.589827000	1.732202000	-0.362651000
1	1.084267000	2.387479000	-0.191614000
1	3.078431000	-0.855351000	-0.681960000
1	2.308236000	1.101608000	-1.408661000
1	-4.127336000	1.931801000	-0.822786000
1	2.467019000	-1.941282000	0.183008000
1	-0.054012000	-3.083355000	0.079274000
1	-3.274545000	0.198640000	1.558932000

#### 10w-IV

8	-1.029712000	-2.142852000	0.824944000
8	0.791547000	-2.543919000	-1.157844000
8	1.309777000	-4.770414000	0.180354000
8	2.364940000	-0.864739000	-0.096003000
8	2.688184000	-2.964918000	1.718566000
8	0.587187000	-2.685153000	3.382226000
8	4.909710000	-1.554319000	-1.265302000
8	3.085126000	-3.274083000	-2.675695000
8	3.778303000	-5.494500000	-1.123409000
8	5.265215000	-3.749426000	0.523609000
1	1.428305000	-2.771536000	2.858892000
1	-0.359972000	-2.254388000	0.092135000
1	1.890045000	-0.058881000	0.139617000
1	1.681103000	-1.446360000	-0.611326000
1	1.016915000	-4.036010000	-0.433963000
1	0.267344000	-2.372285000	-1.952368000
1	2.253395000	-3.669786000	1.171436000
1	2.619732000	-2.164247000	1.149640000
1	3.761246000	-2.647383000	-2.343786000
1	3.576477000	-4.798621000	-1.790976000
1	4.535302000	-3.506096000	1.121969000
1	4.133754000	-1.141044000	-0.842680000
1	5.152713000	-2.268500000	-0.632694000
1	2.278400000	-3.020199000	-2.169673000
1	4.845847000	-4.442402000	-0.036360000
1	2.937448000	-5.533790000	-0.631249000
1	0.518642000	-4.962049000	0.723607000
1	-0.497843000	-1.945959000	1.612634000
1	0.870723000	-2.394623000	4.256794000
8	-0.982767000	-4.741373000	1.921933000
1	-0.508696000	-4.359723000	2.680398000
1	-1.228137000	-3.919639000	1.441969000

#### 10w-V

8	-0.893233000	-1.739503000	0.655930000
8	0.644742000	-2.639351000	-1.143048000
8	1.259817000	-4.749475000	0.402408000
8	2.338334000	-0.795490000	-0.208476000
8	3.005112000	-3.435213000	-2.562068000
8	3.806340000	-5.493153000	-0.853133000
8	2.886493000	-2.783259000	1.696732000
8	4.829652000	-1.557780000	-1.443044000
8	5.417419000	-3.567903000	0.493103000
8	0.196540000	-3.284921000	2.796051000
1	1.123155000	-2.998512000	2.689188000
1	-0.315313000	-2.121024000	-0.132278000
1	1.775973000	-0.132935000	0.233942000
1	1.688916000	-1.394101000	-0.676432000
1	0.946089000	-4.065350000	-0.252609000
1	0.184305000	-2.621613000	-1.993939000
1	2.488234000	-3.525913000	1.193490000
1	2.750019000	-2.022150000	1.087031000
1	3.670822000	-2.757020000	-2.315875000
1	3.555241000	-4.856122000	-1.561710000
1	4.715673000	-3.276604000	1.106166000
1	4.099528000	-1.095442000	-0.991288000
1	5.147766000	-2.197953000	-0.769188000
1	2.203689000	-3.152883000	-2.069248000
1	4.979716000	-4.322706000	0.041020000
1	2.994124000	-5.514440000	-0.316935000
1	0.699106000	-4.601234000	1.184271000
1	-0.274427000	-2.734024000	2.139199000
8	0.329654000	0.613822000	1.371132000
1	0.615876000	0.424026000	2.274273000
1	-0.217073000	-0.172597000	1.136551000
1	-1.811909000	-1.849712000	0.383507000

**OH(H<sub>2</sub>O)<sub>11</sub>****11w-I**

8	0.193896000	-1.184367000	-1.665043000
8	0.464125000	0.409355000	0.359161000
8	2.652671000	-0.332762000	-2.441472000
8	0.605990000	-2.978264000	-3.703066000
8	1.282461000	-5.140576000	-2.359635000
8	3.685233000	-2.407811000	-0.902480000
8	3.129930000	-2.160621000	-4.603643000
8	1.085522000	-3.221131000	-0.182456000
8	4.057059000	-4.308934000	-2.942662000
8	3.080405000	1.379691000	-0.251182000
8	4.157436000	-0.705441000	1.355609000
8	1.515880000	-1.533938000	2.141618000
1	-0.696263000	-0.990092000	-1.991471000
1	-0.376441000	0.863286000	0.491246000
1	0.314190000	-0.204352000	-0.450952000
1	4.207621000	-1.340815000	0.613041000
1	3.320397000	-0.980861000	1.784747000
1	4.080612000	-3.711502000	-2.163443000
1	1.039492000	-4.024088000	-0.732476000
1	0.623287000	-2.520972000	-0.727169000
1	2.150619000	1.247060000	0.017587000
1	3.555208000	0.756668000	0.343011000
1	1.697805000	-0.531399000	-2.253823000
1	2.876553000	0.381846000	-1.803450000
1	3.156646000	-1.415201000	-3.973336000
1	3.568569000	-2.892006000	-4.118875000
1	1.428396000	-2.675156000	-4.151388000
1	0.465905000	-2.303666000	-2.987370000
1	1.371948000	-2.297375000	1.552679000
1	1.072491000	-0.814924000	1.646997000
1	2.823458000	-2.741325000	-0.562763000
1	3.393182000	-1.667046000	-1.485926000
1	0.979776000	-4.364650000	-2.923650000
1	0.739827000	-5.884809000	-2.645382000
1	3.219305000	-4.786434000	-2.804888000

**11w-II**

8	0.131920000	-0.779352000	-1.498808000
8	1.587353000	1.408631000	-1.559666000
8	-2.045006000	0.867787000	-1.473383000
8	2.485221000	-2.053927000	-1.128647000
8	2.391178000	-2.493705000	1.458066000
8	-0.082896000	-0.985181000	1.125393000
8	1.465645000	1.322315000	1.220345000
8	-2.355015000	0.824782000	1.290225000
8	-0.718345000	3.089171000	1.290741000
8	-0.535541000	3.387558000	-1.360543000
8	3.919519000	0.004439000	1.696374000
8	4.182159000	0.216334000	-1.157693000
1	-0.193771000	-1.332452000	-2.222736000
1	-1.657933000	1.748760000	-1.615820000
1	-1.254806000	0.260838000	-1.504108000
1	0.122958000	2.598889000	1.420005000
1	-1.382120000	2.365573000	1.388867000
1	3.108757000	0.556849000	1.684199000
1	0.581385000	-1.642542000	1.400206000
1	-0.693430000	4.306415000	-1.605053000
1	-0.625106000	3.361394000	-0.364423000
1	1.020329000	0.585344000	-1.684392000
1	0.981169000	2.156654000	-1.705954000
1	3.430606000	0.802988000	-1.366085000
1	4.211802000	0.215214000	-0.177352000
1	3.154043000	-1.346244000	-1.256068000
1	1.616343000	-1.590777000	-1.307187000
1	-1.705467000	0.122417000	1.478346000
1	-2.385619000	0.809124000	0.304574000
1	0.895547000	0.517554000	1.282689000
1	1.581581000	1.404705000	0.243499000
1	2.459014000	-2.397753000	0.456719000
1	2.600698000	-3.418161000	1.635253000
1	3.550451000	-0.895402000	1.762613000
1	-0.077775000	-1.033803000	0.121184000

**11w-III**

8	0.212290000	-1.128104000	-1.654870000
8	0.496359000	0.419762000	0.386427000
8	2.636554000	-0.333502000	-2.453002000

8	0.524040000	-2.954672000	-3.759055000
8	1.316849000	-5.152941000	-2.276846000
8	3.587909000	-2.438955000	-0.983643000
8	3.142092000	-2.111571000	-4.625772000
8	1.068132000	-3.224168000	-0.212042000
8	4.117466000	-4.269816000	-2.845608000
8	3.110241000	1.351499000	-0.253843000
8	4.179395000	-0.786678000	1.307929000
8	1.551099000	-1.566445000	2.109601000
1	-0.660533000	-0.916164000	-2.015249000
1	-0.339391000	0.875684000	0.540406000
1	0.330564000	-0.181110000	-0.435788000
1	4.200164000	-1.407111000	0.553609000
1	3.338237000	-1.047052000	1.741603000
1	4.009938000	-3.617381000	-2.098309000
1	1.055780000	-4.011256000	-0.799238000
1	0.604967000	-2.515007000	-0.740296000
1	2.181617000	1.229422000	0.026503000
1	3.583692000	0.715258000	0.325995000
1	1.675202000	-0.523125000	-2.254708000
1	2.874973000	0.380284000	-1.819203000
1	3.125427000	-1.381897000	-3.975228000
1	3.593167000	-2.833784000	-4.152551000
1	1.345285000	-2.668902000	-0.208450000
1	0.428241000	-2.298712000	-3.027191000
1	1.377153000	-2.321342000	1.516619000
1	1.104165000	-0.834609000	1.636571000
1	2.720857000	-2.749949000	-0.617558000
1	3.309466000	-1.664000000	-1.536125000
1	0.970097000	-4.458772000	-2.887797000
1	2.271956000	-5.121064000	-2.458127000
1	5.012993000	-4.614623000	-2.748459000

**11w-IV**

8	0.000446000	-0.002091000	-1.998474000
8	-0.170674000	1.968147000	-0.264306000
8	0.169805000	-1.966501000	-0.261260000
8	2.716723000	0.173195000	-1.814275000
8	3.045933000	-1.896904000	0.244356000
8	-2.716594000	-0.172339000	-1.816803000
8	-0.000783000	0.001080000	1.691032000
8	-2.710445000	-2.199640000	0.082560000
8	-2.793438000	-0.139073000	1.967091000
8	-3.045083000	1.895047000	0.244444000
8	2.792768000	0.137925000	1.966105000
8	2.710405000	2.201107000	0.082868000
1	0.000190000	-0.004891000	-2.966084000
1	-2.954421000	0.603543000	-1.280449000
1	-1.725193000	-0.100339000	-1.900327000
1	-1.820032000	-0.080619000	-2.085297000
1	-2.870706000	-0.932562000	1.385465000
1	1.819648000	0.080593000	2.086481000
1	1.113470000	-2.189219000	-0.175231000
1	-3.755272000	2.483229000	0.524869000
1	-3.018752000	1.169022000	0.931661000
1	-0.125286000	1.317061000	-1.031782000
1	-1.115449000	2.186262000	-0.177704000
1	1.755513000	2.395588000	0.052595000
1	1.725580000	0.099945000	-1.899186000
1	-1.755321000	-2.393117000	0.051951000
1	-2.807218000	-1.561814000	-0.663830000
1	0.032674000	-0.762806000	1.064331000
1	-0.033064000	0.764288000	1.063735000
1	3.765462000	-2.477295000	0.517177000
1	0.126165000	-1.316153000	-1.030153000
1	2.954635000	-0.603566000	-1.279191000
1	2.806437000	1.562973000	-0.663341000
1	2.869585000	0.931741000	1.384984000
1	3.018856000	-1.171501000	0.932015000

**11w-V**

8	-0.181634000	-0.200585000	-2.076033000
8	-2.741417000	-0.134154000	-1.726173000
8	0.047131000	-2.061477000	-0.107230000
8	-0.013178000	1.876335000	-0.449123000
8	2.592295000	-0.118665000	-1.847072000
8	2.858272000	-2.121247000	0.122086000
8	0.123644000	0.046881000	1.703499000
8	2.614323000	2.202162000	-0.017423000

8	-2.730631000	2.061534000	0.090657000
8	2.920005000	0.053462000	2.051722000
8	-2.802018000	-1.993925000	0.422468000
8	-2.677982000	0.219207000	2.236454000
1	-0.070311000	-0.228087000	-3.036955000
1	-3.166766000	-0.313439000	-2.572960000
1	-1.730971000	-0.175207000	-1.916934000
1	-1.700282000	0.199003000	2.278177000
1	-2.857327000	-0.593752000	1.717528000
1	1.940018000	0.040207000	2.110167000
1	1.005002000	-2.267040000	-0.017685000
1	-0.003532000	-1.499914000	-0.924752000
1	-2.915963000	1.408262000	-0.612505000
1	-2.799162000	1.510552000	0.903669000
1	-0.081166000	1.176595000	-1.166315000
1	-0.947709000	2.120293000	-0.249814000
1	1.631097000	2.236293000	-0.130441000
1	2.760104000	0.688252000	-1.329291000
1	1.605307000	-0.141317000	-1.915607000
1	-1.863656000	-2.255740000	0.368176000
1	-2.897438000	-1.426661000	-0.369355000
1	0.056676000	-0.763990000	1.143033000
1	0.103313000	0.751595000	1.018404000
1	2.896086000	-1.506254000	-0.642861000
1	2.986247000	-1.502515000	0.869712000
1	3.064364000	0.809556000	1.457561000
1	2.915574000	3.097080000	-0.211603000

**OH(H<sub>2</sub>O)<sub>12</sub>**

**12w-I**

8	-0.084386000	0.918099000	2.094427000
8	-0.411821000	3.086346000	0.631777000
8	-0.095793000	-1.600167000	1.354550000
8	-2.632395000	0.881122000	1.199380000
8	0.120607000	-1.116451000	-1.348360000
8	2.900441000	-1.577284000	-1.606801000
8	-2.704654000	1.253386000	-1.554939000
8	2.536101000	0.750077000	1.400358000
8	3.034771000	1.303070000	-1.118678000
8	0.264715000	1.664709000	-1.618387000
8	-2.938234000	-2.011032000	0.873463000
8	2.724733000	-2.079238000	1.215279000
8	-2.614329000	-1.549306000	-1.741074000
1	-0.076092000	1.056860000	3.052147000
1	-2.908742000	-0.050238000	1.250916000
1	-1.709679000	0.874526000	1.582246000
1	-1.630592000	-1.544427000	-1.753478000
1	-2.802000000	-0.585021000	-1.799415000
1	1.923658000	-1.513610000	-1.673644000
1	-1.375915000	3.167175000	0.621531000
1	-0.255618000	2.321359000	1.268733000
1	1.242620000	1.659594000	-1.628116000
1	0.050492000	2.212294000	-0.822712000
1	-3.593450000	-2.703824000	1.014444000
1	-2.878934000	-1.903331000	-0.119039000
1	-0.109956000	-0.654758000	1.715032000
1	-1.022277000	-1.897946000	1.384682000
1	1.756761000	-2.157083000	1.314188000
1	2.852673000	-2.035834000	0.243918000
1	2.689512000	-0.217953000	1.458932000
1	1.581126000	0.856660000	1.668814000
1	-1.789761000	1.444360000	-1.821979000
1	-2.651591000	1.199376000	-0.570929000
1	0.116135000	-0.133005000	-1.411977000
1	0.078314000	-1.283590000	-0.374905000
1	2.852204000	1.144248000	-0.139669000
1	3.706108000	1.995282000	-1.134993000
1	3.156963000	-0.637772000	-1.572693000

**12w-II**

8	-0.240953000	1.445931000	1.821113000
8	-0.172940000	-1.211951000	1.747705000
8	0.149482000	3.269099000	-0.050390000
8	-2.659150000	1.207352000	0.910042000
8	2.436090000	1.149034000	1.162046000
8	2.936127000	0.862465000	-1.557125000
8	0.199166000	1.236574000	-1.967819000
8	0.163498000	-1.347859000	-0.938116000

8	-2.693925000	0.692704000	-1.886556000
8	-2.579069000	-2.107722000	-1.392290000
8	-2.935488000	-1.612062000	1.389316000
8	2.720247000	-2.051296000	-1.154572000
8	2.640351000	-1.667263000	1.766499000
1	-0.244049000	1.775273000	2.731178000
1	-1.722577000	1.341618000	1.295983000
1	-1.604678000	-2.064606000	-1.332079000
1	-2.777476000	-1.192112000	-1.683695000
1	1.742321000	-1.849330000	-1.149203000
1	1.089932000	3.483166000	0.020764000
1	-0.001842000	2.644377000	0.722187000
1	1.177040000	1.137253000	-2.026958000
1	0.108792000	1.982288000	-1.329333000
1	-2.912508000	-1.889622000	0.446883000
1	-0.204333000	-0.214523000	1.858208000
1	-1.117179000	-1.485364000	1.778418000
1	1.669540000	-1.706050000	1.876489000
1	2.774101000	-1.943183000	0.841789000
1	2.643885000	0.245334000	1.475506000
1	1.482457000	1.253909000	1.404957000
1	-1.781991000	0.879581000	-2.170793000
1	-2.679026000	0.936590000	-0.937136000
1	0.094284000	-0.414267000	-1.250139000
1	0.047952000	-1.284635000	0.046432000
1	2.798407000	1.023022000	-0.592246000
1	3.081838000	-0.098974000	-1.588231000
1	2.805909000	-2.860540000	-1.672272000
1	-3.126659000	2.025903000	1.116276000
1	-3.051655000	-0.645138000	1.318195000

**12w-III**

8	0.108100000	1.280796000	-1.909289000
8	-0.193247000	3.230353000	-0.183031000
8	0.221152000	-1.398457000	-1.609514000
8	2.568414000	1.229290000	-1.045261000
8	-0.019206000	-1.393356000	1.129079000
8	-2.751527000	-2.019608000	1.317280000
8	2.717393000	0.953541000	1.781748000
8	-2.497978000	0.854754000	-1.214572000
8	-2.999595000	0.905382000	1.378327000
8	-0.220419000	1.357296000	1.886877000
8	3.013604000	-1.605775000	-1.307111000
8	-2.590705000	-1.929963000	-1.541355000
8	2.779350000	-1.896550000	1.505894000
1	0.092616000	1.520625000	-2.846847000
1	2.973762000	2.061939000	-1.316571000
1	1.619428000	1.277416000	-1.410783000
1	1.801433000	-1.928526000	1.489780000
1	2.923045000	-0.952118000	1.723703000
1	-1.775750000	-1.923472000	1.380557000
1	-1.110015000	3.520278000	-0.277107000
1	-0.087696000	2.544701000	-0.915938000
1	-1.186419000	1.246186000	1.974247000
1	-0.156139000	2.045460000	1.183672000
1	3.074994000	-0.632052000	-1.316807000
1	3.032071000	-1.807029000	-0.344647000
1	0.187555000	-0.418365000	-1.793178000
1	1.180281000	-1.613414000	-1.639655000
1	-1.623080000	-1.985614000	-1.662607000
1	-2.709931000	-2.098695000	-0.582241000
1	-2.630710000	-0.095453000	-1.436661000
1	-1.552413000	1.021215000	-1.475094000
1	1.804979000	1.100762000	2.083754000
1	2.653556000	1.106702000	0.815658000
1	-0.008681000	-0.438612000	1.353904000
1	0.043075000	-1.396712000	0.142000000
1	-2.816186000	0.931786000	0.389735000
1	-3.768461000	1.473665000	1.504575000
1	-3.044003000	-1.102291000	1.463978000

**12w-IV**

1	2.809786000	-1.166248000	-1.085994000
1	2.831207000	-1.160288000	1.051941000
1	2.809750000	1.166253000	1.085961000
1	2.831239000	1.160185000	-1.051993000
8	3.333410000	-0.000026000	0.000022000
8	2.426018000	-1.864637000	-1.693195000

8	2.465300000	-1.908048000	1.618744000
8	2.426035000	1.864667000	1.693167000
8	2.465327000	1.907968000	-1.618753000
1	2.472397000	-2.666784000	-1.155152000
1	2.677014000	-1.644093000	2.522940000
1	2.472441000	2.666800000	1.155106000
1	2.676999000	1.644007000	-2.522956000
1	0.647724000	-1.420499000	-1.772537000
1	0.656191000	-1.804112000	1.354827000
1	0.647733000	1.420617000	1.772548000
1	0.656217000	1.804094000	-1.354809000
8	-0.286858000	-1.168120000	-1.602408000
8	-0.278151000	-1.578203000	1.152704000
8	-0.286837000	1.168188000	1.602425000
8	-0.278138000	1.578252000	-1.152674000
1	-0.272444000	-0.184984000	-1.542425000
1	-0.302683000	-1.518409000	0.169493000
1	-0.272359000	0.185059000	1.542403000
1	-0.302651000	1.518464000	-0.169461000
1	-2.227606000	-1.495581000	-1.666389000
1	-2.221439000	-1.662713000	1.497913000
1	-2.227610000	1.495569000	1.666361000
1	-2.221436000	1.662716000	-1.497910000
8	-3.171265000	-1.343039000	-1.479919000
8	-3.165937000	-1.480546000	1.346705000
8	-3.171268000	1.343027000	1.479893000
8	-3.165928000	1.480521000	-1.346702000
1	-3.234686000	-1.492363000	-0.510053000
1	-3.233117000	-0.510531000	1.494833000
1	-3.234684000	1.492335000	0.510023000
1	-3.233076000	0.510502000	-1.494780000
1	4.301432000	-0.000021000	0.000038000

**12w-V**

1	-0.208073000	0.018874000	2.794950000
8	0.063619000	0.024060000	1.865825000
8	-3.835918000	-1.660328000	1.191820000
1	-3.464274000	-1.879128000	0.298067000
1	-3.356494000	-2.253826000	1.784119000
8	3.225932000	-0.318615000	-1.950590000
1	2.292451000	-0.088461000	-2.128033000
1	3.466640000	0.350040000	-1.274394000
8	2.600282000	-0.563242000	1.987586000
1	1.603429000	-0.335857000	1.983955000
1	2.842876000	-0.620175000	2.919273000
8	0.725946000	2.148344000	0.351212000
1	-0.063061000	2.719630000	0.267092000
1	0.469765000	1.464097000	1.029169000
8	-1.893214000	3.333335000	-0.008315000
1	-2.071963000	3.041055000	-0.916126000
1	-2.244892000	2.578313000	0.506265000
8	-2.384113000	0.775646000	-1.838122000
1	-2.403612000	0.776148000	-0.856349000
1	-1.423807000	0.693129000	-2.021155000
8	-0.072076000	-1.832375000	-0.095388000
1	-0.074217000	-1.271557000	0.724984000
1	0.838792000	-2.206501000	-0.136700000
8	0.419713000	0.353876000	-1.789297000
1	0.245513000	-0.452412000	-1.250316000
1	0.580010000	1.037473000	-1.098003000
8	2.646549000	-2.439622000	-0.164793000
1	2.930111000	-1.798973000	-0.855736000
1	2.787754000	-1.9311617000	0.657178000
8	3.524617000	1.493551000	0.245079000
1	3.345901000	0.814490000	0.925904000
1	2.673416000	1.969852000	0.217695000
8	-2.385428000	0.772260000	0.993469000
1	-2.977753000	0.018055000	1.191082000
1	-1.484260000	0.467140000	1.296910000
8	-2.628885000	-2.063600000	-1.227884000
1	-1.702754000	-2.122036000	-0.910081000
1	-2.657692000	-1.174080000	-1.634572000

**OH(H<sub>2</sub>O)<sub>13</sub>**

**13w-I**

8	-0.215290000	-0.702822000	-2.040073000
8	-1.014091000	-2.745824000	-0.467263000
8	0.689432000	1.685447000	-1.435711000

8	-2.463975000	0.208101000	-1.051157000
8	0.801520000	1.189815000	1.269917000
8	3.592919000	0.735927000	1.484927000
8	-2.557846000	-0.138902000	1.704317000
8	2.336385000	-1.424811000	-1.386106000
8	2.753660000	-2.040079000	1.138615000
8	0.029961000	-1.461914000	1.677428000
8	-1.854296000	3.021962000	-0.862451000
8	3.508773000	1.165176000	-1.353570000
8	-1.574366000	2.544096000	1.762462000
1	-0.291540000	-0.870039000	-2.990330000
1	-2.446256000	1.172787000	-1.177552000
1	-1.610381000	-0.129666000	-1.482025000
1	-0.656508000	2.187558000	1.722308000
1	-2.082647000	1.718655000	1.908138000
1	2.650636000	0.994660000	1.566407000
1	-1.987496000	-2.692109000	-0.457027000
1	-0.735476000	-2.064656000	-1.138846000
1	0.955421000	-1.775686000	1.708170000
1	-0.352132000	-1.966999000	0.911026000
1	-2.255025000	3.886579000	-1.007906000
1	-1.791352000	2.924728000	0.129738000
1	0.337554000	0.790851000	-1.753284000
1	-0.081481000	2.279143000	-1.448017000
1	2.627890000	1.575889000	-1.438871000
1	3.646895000	1.117307000	-0.383871000
1	2.810329000	-0.572928000	-1.500923000
1	1.396021000	-1.211832000	-1.632897000
1	-1.737875000	-0.590399000	-1.975501000
1	-2.441463000	-0.034747000	0.730115000
1	0.484097000	0.260839000	1.362484000
1	0.795868000	1.343944000	0.293538000
1	2.579132000	-1.860464000	0.162996000
1	3.149415000	-2.919424000	1.158804000
1	3.530528000	-0.236654000	1.491181000
8	-3.911994000	-2.071590000	-0.268860000
1	3.642910000	-1.259647000	-0.742417000
1	-3.817599000	-1.784329000	0.653760000

**13w-II**

1	0.200794000	-0.637091000	-2.660205000
8	0.036606000	-0.669015000	-1.705003000
8	3.836985000	-1.451031000	-0.254875000
1	3.553727000	-1.293964000	0.672055000
1	3.167149000	-2.085775000	-0.581065000
8	1.512510000	-2.949300000	-1.109523000
1	0.973829000	-2.162227000	-1.377891000
1	1.135746000	-3.172663000	-0.246062000
8	-3.538503000	0.552693000	1.761057000
1	-2.675017000	0.978629000	1.924983000
1	-3.702714000	0.769008000	0.817631000
8	-2.414749000	-1.597212000	-1.551595000
1	-1.457160000	-1.273813000	-1.648856000
1	-2.517749000	-2.280911000	-2.224288000
8	-0.925235000	1.810576000	-1.086467000
1	-0.207825000	2.445261000	-1.291814000
1	-0.565039000	0.925480000	-1.366560000
8	1.479407000	3.348543000	-1.369920000
1	1.642313000	3.564657000	-0.438327000
1	1.963465000	2.500834000	-1.455767000
8	2.082189000	1.997416000	1.450901000
1	2.136575000	1.539808000	0.583719000
1	1.128264000	1.953774000	1.664256000
8	0.013773000	-1.233588000	1.120856000
1	0.065035000	-1.045522000	0.164221000
1	-0.894485000	-1.614100000	1.244288000
8	-0.751112000	1.448259000	1.677198000
1	-0.477712000	0.506958000	1.632065000
1	-0.871689000	1.662911000	0.722838000
8	-2.582926000	-2.036357000	1.259324000
1	-3.008106000	-1.189990000	1.531347000
1	-2.677243000	-2.023138000	0.286513000
8	-3.646319000	0.965546000	-1.054500000
1	-3.384797000	0.071702000	-1.346331000
1	-2.817561000	1.469026000	-1.171061000
8	2.320924000	0.718446000	-1.060489000
1	2.999723000	0.026653000	-0.878264000
1	1.508048000	0.194726000	-1.277479000
8	2.635660000	-0.777053000	2.240442000

1	1.729090000	-1.050225000	2.004361000
1	2.579656000	0.196610000	2.176447000

**13w-III**

1	-0.277263000	-1.517019000	2.316445000
8	-0.176225000	-1.293659000	1.378540000
8	0.942862000	1.967969000	-1.121623000
1	0.162538000	2.570676000	-1.168237000
1	0.572817000	1.096426000	-1.373500000
8	2.231609000	-2.260687000	0.903803000
1	2.233641000	-3.181965000	1.190277000
1	1.294643000	-1.929926000	1.100571000
8	-2.553352000	0.046044000	1.195378000
1	-3.210865000	-0.642583000	0.971437000
1	-1.696693000	-0.453009000	1.277117000
8	0.013266000	-0.700784000	-1.428190000
1	-0.032182000	-0.858715000	-0.465654000
1	0.918386000	-1.026003000	-1.679760000
8	-2.561608000	0.604755000	-1.560902000
1	-1.733364000	0.156662000	-1.813255000
1	-2.545713000	0.514324000	-0.581879000
8	0.910247000	1.262383000	1.597441000
1	0.969394000	1.557914000	0.660311000
1	0.509910000	0.357890000	1.532683000
8	3.663700000	1.011476000	-1.185785000
1	2.858142000	1.558219000	-1.237450000
1	3.749921000	0.828123000	-0.224991000
8	-1.483563000	3.290393000	-1.010202000
1	-1.584834000	3.206029000	-0.035924000
1	-1.983895000	2.521165000	-1.344506000
8	-1.494593000	-3.144007000	-0.157881000
1	-1.024765000	-2.539248000	0.475853000
1	-1.085196000	-2.904821000	-1.002887000
8	2.576320000	-1.483687000	-1.817572000
1	2.614728000	-1.876226000	-0.922984000
1	3.048891000	-0.625879000	-1.702896000
8	-1.600414000	2.687682000	1.762815000
1	-0.701144000	2.317555000	1.874818000
1	-2.141426000	1.877822000	1.713305000
8	-4.024011000	-1.891978000	-0.290598000
1	-3.859358000	-1.259966000	-1.009672000
1	-3.205764000	-2.436966000	-0.287138000
8	3.572203000	0.241160000	1.553270000
1	2.716906000	0.682234000	1.741668000
1	3.301019000	-0.689209000	1.448314000

**13w-IV**

1	-0.335068000	-1.504486000	2.332780000
8	-0.212864000	-1.284372000	1.396591000
8	-4.044623000	-1.858973000	-0.309821000
1	-3.868740000	-1.232229000	-1.030958000
1	-3.229503000	-2.408925000	-0.297166000
8	-1.525363000	-3.123581000	-0.158274000
1	-1.055489000	-2.524695000	0.480555000
1	-1.104882000	-2.886396000	-0.998556000
8	3.779294000	0.893534000	-1.211223000
1	2.958917000	1.417785000	-1.299997000
1	3.830931000	0.761884000	-0.240123000
8	2.218258000	-2.201203000	1.006073000
1	1.264737000	-1.894934000	1.168330000
1	2.259659000	-3.092449000	1.373066000
8	0.791298000	1.282980000	1.579976000
1	0.011018000	1.854647000	1.771405000
1	0.415074000	0.365690000	1.548878000
8	-1.598510000	2.710513000	1.713712000
1	-1.610022000	3.030840000	0.784949000
1	-2.149964000	1.907516000	1.667293000
8	-1.468710000	3.277681000	-1.076030000
1	-1.953192000	2.496156000	-1.405685000
1	-0.537693000	2.996832000	-1.185190000
8	0.027355000	-0.729086000	-1.449820000
1	-0.033757000	-0.841492000	-0.482312000
1	0.933020000	-1.074864000	-1.667256000
8	1.079607000	1.935090000	-1.102382000
1	0.692863000	1.095403000	-1.423450000
1	1.047700000	1.783248000	-0.127076000
8	2.589197000	-1.581471000	-1.748687000

1	3.101652000	-0.743470000	-1.662461000
1	2.604157000	-1.937733000	-0.838377000
8	3.496421000	0.334277000	1.572808000
1	3.190994000	-0.590031000	1.507554000
1	2.667348000	0.818866000	1.749520000
8	-2.574334000	0.073661000	1.182451000
1	-3.239749000	-0.605982000	0.953638000
1	-1.726331000	-0.438157000	1.270637000
8	-2.543023000	0.594130000	-1.584759000
1	-1.713847000	0.143652000	-1.830208000
1	-2.531879000	0.517874000	-0.604725000

**13w-V**

1	-0.431656000	1.323261000	2.422976000
8	-0.241872000	1.119755000	1.494460000
8	-1.437065000	-2.977250000	-1.290244000
1	-1.988336000	-2.211140000	-1.527168000
1	-0.526089000	-2.675208000	-1.466303000
8	-2.594963000	-0.373197000	1.222322000
1	-2.634321000	-0.528420000	0.256768000
1	-1.766171000	0.158739000	1.321203000
8	3.575120000	-0.478667000	1.410195000
1	3.255840000	0.442738000	1.454409000
1	2.762288000	-0.983482000	1.604136000
8	-1.454666000	3.136322000	0.094398000
1	-0.957924000	3.103061000	-0.735066000
1	-1.008102000	2.444073000	0.652768000
8	-3.980874000	1.846560000	-0.225155000
1	-3.844460000	1.231152000	0.516340000
1	-3.181203000	2.411644000	-0.159994000
8	2.463450000	1.901371000	-1.661779000
1	1.550066000	1.568580000	-1.751756000
1	2.496788000	2.092175000	-0.703561000
8	1.168731000	-1.780097000	-1.184610000
1	2.100699000	-1.535572000	-1.402472000
1	1.144938000	-1.735223000	-0.198407000
8	-2.718253000	-0.299583000	-1.673307000
1	-1.828341000	0.117282000	-1.689935000
1	-3.309617000	0.446633000	-1.446168000
8	0.876118000	-1.410363000	1.534752000
1	0.133118000	-2.040029000	1.688842000
1	0.453670000	-0.514295000	1.580318000
8	-0.109815000	0.615845000	-1.298251000
1	-0.173310000	0.770062000	-0.334385000
1	0.351775000	-0.261128000	-1.347663000
8	2.203225000	2.047616000	1.189755000
1	2.253852000	2.883021000	1.669790000
1	1.252132000	1.724600000	1.332572000
8	3.695736000	-0.697370000	-1.436093000
1	3.813150000	-0.669481000	-0.462173000
1	3.398282000	0.214655000	-1.635740000
8	-1.430399000	-2.961889000	1.585272000
1	-1.976509000	-2.151715000	1.645705000
1	-1.456342000	-3.138409000	0.621248000

**OH(H<sub>2</sub>O)<sub>14</sub>**

**14w-I**

8	0.048672000	-0.793448000	-2.062506000
8	-1.283604000	-2.425461000	-0.616124000
8	2.286543000	-2.104515000	-1.114064000
8	2.250748000	-2.330338000	1.633618000
8	-2.021322000	0.755742000	-1.340914000
8	1.491650000	1.380495000	-1.563016000
8	-2.202544000	0.879377000	1.388726000
8	1.337867000	1.096056000	1.109228000
8	-4.531824000	-0.604528000	-1.547030000
8	-0.239898000	-1.164651000	1.654080000
8	-0.613588000	3.241503000	-1.460839000
8	4.057250000	0.177227000	-1.191363000
8	-3.891859000	-1.372742000	-1.168093000
8	3.768534000	0.197549000	1.750464000
8	-0.518232000	3.265769000	1.417513000
1	-0.015817000	-0.970306000	-3.012079000
1	-2.790155000	0.157334000	-1.455778000
1	-1.248419000	0.197500000	-1.648901000
1	0.235947000	2.642974000	1.434100000
1	-1.261813000	2.650107000	1.560608000
1	-3.733050000	-0.024810000	1.577313000



1	-4.314999000	-1.320862000	2.157253000
1	2.871149000	0.602956000	1.596999000
1	-0.911709000	-3.311007000	-0.718477000
1	-0.736993000	-1.833828000	-1.258442000
1	0.616787000	-1.635713000	1.802219000
1	-0.626999000	-1.642456000	0.885357000
1	-1.283830000	2.537126000	-1.550804000
1	-0.606591000	3.404302000	-0.494018000
1	0.960178000	0.573254000	-1.834123000
1	0.861880000	2.129641000	-1.664801000
1	3.305470000	0.764862000	-1.402825000
1	4.139274000	0.252184000	-0.223867000
1	2.990931000	-1.437307000	-1.243066000
1	1.483936000	-1.651868000	-1.477371000
1	-3.092989000	-1.908021000	-0.990590000
1	-4.234952000	-1.182767000	-0.272510000
1	-1.520673000	0.250473000	1.695297000
1	-2.091101000	0.856804000	0.403019000
1	0.737825000	0.326022000	1.232822000
1	1.403036000	1.193443000	0.120158000
1	2.273561000	-2.329529000	0.643860000
1	2.893238000	-1.634772000	1.857543000
1	4.189735000	0.759977000	2.411186000

**14w-II**

8	-0.125073000	-0.764149000	2.040762000
8	1.188232000	-2.443091000	0.652161000
8	-1.453100000	1.512967000	1.473078000
8	-4.059973000	0.369378000	1.116472000
8	-2.418633000	-1.904829000	1.125950000
8	2.019825000	0.710420000	1.336299000
8	-1.275775000	1.239798000	-1.236346000
8	0.739363000	3.273108000	1.396024000
8	2.263444000	0.773841000	-1.388512000
8	-2.378799000	-2.324819000	-1.466907000
8	0.205476000	-1.210185000	-1.654325000
8	0.716189000	3.274048000	-1.471966000
8	3.823269000	-1.481511000	1.236262000
8	-3.852177000	0.206982000	-1.742450000
8	4.569325000	-0.743822000	-1.456189000
1	-0.075090000	-0.909901000	2.996554000
1	2.762857000	0.086316000	1.479348000
1	1.219791000	0.189016000	1.632862000
1	-0.073349000	2.695987000	-1.518597000
1	1.427251000	2.619964000	-1.601672000
1	3.776693000	-0.157823000	-1.520008000
1	4.387313000	-1.444740000	-2.094639000
1	-2.994313000	0.682463000	-1.712056000
1	0.829093000	-3.326529000	0.803194000
1	0.646374000	-1.824372000	1.280820000
1	-0.653293000	-1.658942000	-1.794954000
1	0.570246000	-1.677684000	-0.868071000
1	1.371793000	2.538499000	1.508696000
1	0.758832000	3.421880000	0.426385000
1	-0.969619000	0.688511000	1.758161000
1	-0.786839000	2.230081000	1.572478000
1	-3.312800000	0.966324000	1.313499000
1	-3.076348000	-1.178664000	1.225230000
1	-1.579934000	-1.508107000	1.487370000
1	3.005681000	-1.980384000	1.038947000
1	4.198636000	-1.309357000	0.350018000
1	1.556811000	0.180837000	-1.705635000
1	2.122707000	0.777253000	-0.406371000
1	-0.729661000	0.433657000	-1.334534000
1	-1.367527000	1.333399000	-0.253714000
1	-2.384300000	-2.210982000	-0.464619000
1	-3.555264000	-0.718455000	-1.802783000
1	-4.122668000	0.396118000	0.138247000
1	-2.645816000	-3.239448000	-1.616682000

**14w-III**

8	0.212311000	-1.054920000	-1.954581000
8	-1.172414000	-2.524448000	-0.346273000
8	1.475397000	1.345641000	-1.590843000
8	4.056152000	0.184135000	-1.049611000
8	-1.970411000	0.505275000	-1.407985000
8	-0.732487000	3.065555000	-1.770657000
8	-2.282485000	0.927204000	1.294506000
8	1.235843000	1.465327000	1.154674000

8	-3.789186000	-1.634205000	-1.084416000
8	2.378685000	-2.159422000	-1.018373000
8	2.360307000	-1.980587000	1.855095000
8	-4.571145000	-0.598523000	1.482454000
8	-0.191265000	-0.941510000	1.807471000
8	-0.788506000	3.457710000	1.057719000
8	3.815019000	0.419305000	1.796950000
1	0.104822000	-1.236705000	-2.899593000
1	-2.706907000	-0.140414000	-1.477769000
1	-1.164040000	-0.037102000	-1.616992000
1	0.007824000	2.903609000	1.200533000
1	-1.492739000	2.818125000	1.269246000
1	-3.781970000	-0.004210000	1.502884000
1	-4.407949000	-1.220807000	2.202349000
1	2.983075000	0.932009000	1.737749000
1	4.080886000	0.381171000	0.854096000
1	-0.770423000	-3.400564000	-0.293081000
1	-0.620091000	-2.019114000	-1.040521000
1	0.699093000	-1.341138000	1.969354000
1	-0.557861000	-1.502396000	1.091468000
1	-1.355359000	2.315301000	-1.799107000
1	-0.779728000	3.343223000	-0.829912000
1	1.018470000	0.487563000	-1.791430000
1	0.794655000	2.031548000	-1.779741000
1	3.346294000	0.789596000	-1.335835000
1	3.605688000	-0.681498000	-1.095123000
1	2.597926000	-2.915024000	-1.576553000
1	1.542168000	-1.753206000	-1.433389000
1	-2.990472000	-2.128234000	-0.814629000
1	-4.177676000	-1.357732000	-0.229935000
1	-1.567754000	0.396216000	1.696002000
1	-2.117468000	0.809826000	0.325550000
1	0.704924000	0.663724000	1.342033000
1	1.368125000	1.418201000	0.176278000
1	2.398878000	-2.167794000	0.897140000
1	2.951084000	-1.196474000	1.939878000

**14w-IV**

8	0.113864000	-0.820776000	-2.053714000
8	-1.267345000	-2.426074000	-0.600237000
8	1.529652000	1.316583000	-1.457975000
8	4.001745000	0.324201000	-1.114927000
8	-1.985325000	0.742899000	-1.398454000
8	-0.512947000	3.198432000	-1.455464000
8	-2.254214000	0.878639000	1.339882000
8	1.271261000	1.184993000	1.291094000
8	-3.856250000	-1.381790000	-1.250446000
8	2.328218000	-2.132878000	-1.102895000
8	2.207034000	-2.304322000	1.704480000
8	-4.586265000	-0.597680000	1.429884000
8	-0.285875000	-1.153110000	1.722871000
8	-0.617209000	3.310826000	1.389831000
8	3.811411000	0.077815000	1.837973000
1	0.054256000	-0.986333000	-3.005504000
1	-2.751791000	0.142503000	-1.521477000
1	-1.207507000	0.178460000	-1.673279000
1	0.141095000	2.697960000	1.489371000
1	-1.361598000	2.693313000	1.515921000
1	-3.785029000	-0.022457000	1.482710000
1	-4.398705000	-1.305812000	2.059062000
1	2.969457000	0.579452000	1.793184000
1	4.119550000	0.137556000	0.916801000
1	-0.893902000	-3.314132000	-0.668808000
1	-0.703602000	-1.853764000	-1.236358000
1	0.581538000	-1.609501000	1.865303000
1	-0.651079000	-1.619763000	0.939236000
1	-1.199437000	2.515327000	-1.579611000
1	-0.569944000	3.381831000	-0.491917000
1	0.990515000	0.517878000	-1.753068000
1	0.919715000	2.084402000	-1.563956000
1	3.171634000	0.828800000	-1.304770000
1	4.642209000	0.651711000	-1.756867000
1	3.027861000	-1.462744000	-1.191975000
1	1.530451000	-1.674930000	-1.475235000
1	-3.064458000	-1.915407000	-1.039766000
1	-4.230780000	-1.185365000	-0.368601000
1	-1.572610000	0.267169000	1.674730000
1	-2.103540000	0.850927000	0.355045000
1	0.696343000	0.399025000	1.414929000

1	1.385120000	1.220366000	0.311350000
1	2.238463000	-2.357388000	0.722360000
1	2.843717000	-1.581153000	1.883158000

#### 14w-V

8	0.151861000	-0.820567000	-2.004814000
8	-1.166920000	-2.455102000	-0.577929000
8	2.392705000	-2.007055000	-1.015763000
8	2.349123000	-2.200234000	1.598754000
8	-2.005931000	0.657306000	-1.359662000
8	1.566247000	1.455517000	-1.485623000
8	-2.297196000	0.821520000	1.346060000
8	1.206565000	1.358824000	1.296539000
8	-4.608020000	-0.697159000	1.411574000
8	-0.236466000	-1.113803000	1.682527000
8	-0.703590000	3.208201000	-1.502519000
8	4.126832000	0.190017000	-1.156685000
8	-3.799172000	-1.543492000	-1.235306000
8	3.817355000	0.324572000	1.700482000
8	-0.751219000	3.302203000	1.314140000
1	0.105702000	-0.993598000	-2.956282000
1	-2.737879000	0.020949000	-1.505282000
1	-1.192668000	0.141556000	-1.633976000
1	-1.450992000	2.638745000	1.462194000
1	-3.819422000	-0.106473000	1.476437000
1	-4.444421000	-1.371990000	2.082287000
1	2.998959000	0.859280000	1.697500000
1	3.465422000	-0.576136000	1.820961000
1	-0.792267000	-3.338471000	-0.686252000
1	-0.622358000	-1.853871000	-1.224585000
1	0.622565000	-1.546510000	1.865641000
1	-0.576167000	-1.617765000	0.907073000
1	-1.347218000	2.482864000	-1.610839000
1	1.068439000	0.633817000	-1.743353000
1	3.369946000	0.760182000	-1.406052000
1	4.168013000	0.306403000	-0.184183000
1	3.087776000	-1.323953000	-1.160282000
1	1.575716000	-1.589422000	-1.404239000
1	-2.981094000	-2.028450000	-1.007083000
1	-4.190091000	-1.339402000	-0.362886000
1	-1.607555000	0.223102000	1.690565000
1	-2.146253000	0.783521000	0.364710000
1	0.656774000	0.554922000	1.388797000
1	2.355595000	-2.176707000	0.589005000
1	2.644641000	-3.088039000	1.832758000
1	1.489701000	1.444284000	-0.505722000
1	0.575054000	2.109528000	1.413965000
1	0.147219000	2.737151000	-1.630075000
1	-0.760539000	3.408506000	0.335004000

#### OH(H<sub>2</sub>O)<sub>15</sub>

##### 15w-I

1	0.024095000	-0.831287000	-2.592988000
8	0.072824000	-0.787514000	-1.625078000
8	-2.338976000	-2.235395000	1.702917000
1	-1.553364000	-1.701727000	1.908727000
1	-2.178307000	-2.464189000	0.764227000
8	-0.006423000	-0.487929000	1.263291000
1	0.642610000	0.251850000	1.381107000
1	-0.027261000	-0.609573000	0.293195000
8	-0.100720000	3.651520000	1.294033000
1	-0.883464000	3.080574000	1.429986000
1	-0.072427000	3.722385000	0.315029000
8	-4.358790000	-0.278622000	1.248781000
1	-3.768271000	0.491268000	1.359774000
1	-3.771727000	-1.014862000	1.522897000
8	1.749115000	1.609342000	1.322654000
1	1.183596000	2.408806000	1.457634000
1	1.837561000	1.561681000	0.340395000
8	-1.801323000	-2.553597000	-1.062756000
1	-1.049282000	-1.914327000	-1.282794000
1	-1.480893000	-3.417875000	-1.349513000
8	-3.976519000	-0.647715000	-1.519951000
1	-4.241574000	-0.531810000	-0.578905000
1	-3.396353000	-1.430008000	-1.486581000
8	-0.014385000	3.368492000	-1.542582000
1	-0.775716000	2.772596000	-1.677487000
1	0.745795000	2.767036000	-1.648367000

8	1.877377000	1.192286000	-1.392404000
1	2.758948000	0.786242000	-1.494882000
1	1.232163000	0.435609000	-1.501147000
8	4.258950000	-0.321010000	-1.088180000
1	5.189914000	-0.216496000	-1.315841000
1	4.220126000	-0.262740000	-0.090126000
8	2.245669000	-2.453794000	-1.197844000
1	3.003324000	-1.856351000	-1.328010000
1	1.461445000	-1.876852000	-1.379372000
8	-1.866540000	1.169449000	-1.479532000
1	-2.687376000	0.644879000	-1.630254000
1	-1.156493000	0.477612000	-1.524817000
8	-2.100227000	1.566470000	1.247223000
1	-2.063974000	1.520869000	0.260716000
1	-1.483601000	0.845192000	1.477632000
8	2.202006000	-2.403904000	1.606669000
1	2.231238000	-2.573160000	0.637461000
1	1.358898000	-1.923027000	1.695962000
8	3.914698000	-0.217308000	1.553913000
1	3.284849000	0.515442000	1.696108000
1	3.361654000	-1.023917000	1.690999000

##### 15w-II

1	-0.006208000	-0.819908000	-2.600819000
8	0.024800000	-0.770356000	-1.632507000
8	-2.225714000	-2.304988000	1.685283000
1	-1.416538000	-1.797054000	1.862746000
1	-2.143494000	-2.498507000	0.722395000
8	0.086796000	-0.478166000	1.262542000
1	0.766542000	0.243140000	1.341014000
1	0.024873000	-0.618146000	0.296753000
8	0.057482000	3.666548000	1.310773000
1	-0.721543000	3.103841000	1.484188000
1	0.056091000	3.723820000	0.330281000
8	-4.129788000	-0.294497000	1.369904000
1	-3.522346000	0.462922000	1.504157000
1	-3.547965000	-1.060288000	1.589332000
8	1.877136000	1.565329000	1.249523000
1	1.344181000	2.379555000	1.408745000
1	1.948083000	1.529598000	0.263742000
8	-2.066362000	-2.481632000	-1.092475000
1	-1.296897000	-1.895339000	-1.308511000
1	-2.837404000	-1.929187000	-1.313353000
8	-4.161629000	-0.441325000	-1.290469000
1	-4.246173000	-0.381745000	-0.294581000
1	-5.064730000	-0.413891000	-1.626995000
8	0.073846000	3.374321000	-1.522270000
1	-0.688499000	2.778147000	-1.640927000
1	0.833814000	2.775139000	-1.652216000
8	1.927072000	1.191916000	-1.467169000
1	2.779257000	0.705028000	-1.560492000
1	1.242963000	0.475783000	-1.549567000
8	4.119520000	-0.505174000	-1.345760000
1	3.572259000	-1.309562000	-1.402301000
1	4.258438000	-0.400882000	-0.376722000
8	1.988937000	-2.495777000	-1.198631000
1	1.711960000	-3.337532000	-1.581069000
1	1.213266000	-1.871418000	-1.365781000
8	-1.825771000	1.195559000	-1.397759000
1	-2.681470000	0.757177000	-1.565415000
1	-1.153688000	0.461542000	-1.484362000
8	-1.959774000	1.551062000	1.351250000
1	-1.953834000	1.535706000	0.364679000
1	-1.309935000	0.842779000	1.537066000
8	2.313584000	-2.378234000	1.629792000
1	2.264466000	-2.562914000	0.670192000
1	1.490262000	-1.875065000	1.763237000
8	4.146520000	-0.211010000	1.457871000
1	3.520383000	0.526085000	1.579592000
1	3.590632000	-0.997420000	1.645805000

##### 15w-III

1	-0.001413000	-0.945369000	-2.552231000
8	-0.013632000	-1.020834000	-1.584760000
8	0.077315000	-0.597178000	1.321069000
1	0.844536000	-1.186855000	1.562091000
1	0.035806000	-0.669123000	0.347641000
8	-1.836148000	1.071372000	-1.336139000
1	-2.718247000	0.638887000	-1.436654000

1	-1.197232000	0.322652000	-1.424295000
8	0.091167000	3.813920000	0.965498000
1	0.854470000	3.240187000	1.173955000
1	-0.657964000	3.243861000	1.228938000
8	-4.218463000	-0.029286000	1.508124000
1	-3.566579000	0.692610000	1.587074000
1	-3.666376000	-0.816211000	1.707681000
8	4.228312000	-0.180686000	1.508122000
1	3.605030000	0.570291000	1.561554000
1	4.345451000	-0.281013000	0.539195000
8	-2.143671000	-2.517568000	-1.120054000
1	-2.006534000	-3.381718000	-1.525780000
1	-1.305667000	-1.990388000	-1.323320000
8	-2.361426000	-2.155597000	1.712023000
1	-1.515710000	-1.673928000	1.786526000
1	-2.344967000	-2.431950000	0.775164000
8	-0.015518000	3.218807000	-1.808859000
1	-0.802658000	2.641267000	-1.799775000
1	0.009337000	3.566097000	-0.889496000
8	1.777929000	1.157105000	-1.477662000
1	1.146506000	0.399774000	-1.498135000
1	1.219759000	1.937415000	-1.719090000
8	4.089093000	-0.528210000	-1.322052000
1	3.466293000	0.192240000	-1.536003000
1	3.509029000	-1.312808000	-1.337160000
8	2.049955000	-2.569026000	-1.071828000
1	1.946183000	-3.395791000	-1.557429000
1	1.230266000	-2.018017000	-1.297996000
8	-4.156670000	-0.421480000	-1.274880000
1	-3.658654000	-1.258945000	-1.300297000
1	-4.316524000	-0.285043000	-0.312440000
8	-1.815542000	1.660566000	1.357702000
1	-1.206828000	0.962832000	1.658852000
1	-1.836457000	1.498338000	0.382982000
8	1.992617000	1.638926000	1.240401000
1	1.323605000	0.973672000	1.491251000
1	2.005727000	1.518515000	0.260433000
8	2.251374000	-2.135902000	1.740771000
1	2.272587000	-2.480873000	0.827297000
1	3.013679000	-1.510047000	1.759656000

**15w-IV**

1	0.018513000	-0.907233000	2.571591000
8	0.040815000	-0.863614000	1.602664000
8	-0.021127000	-0.750396000	-1.314456000
1	-0.765873000	-1.380095000	-1.525002000
1	0.018518000	-0.779557000	-0.338141000
8	1.810430000	1.201216000	1.348381000
1	2.692153000	0.783174000	1.492583000
1	1.176122000	0.444349000	1.464639000
8	-0.140410000	3.691328000	-1.193759000
1	-0.876983000	3.086561000	-1.407583000
1	0.633071000	3.122724000	-1.383367000
8	4.287395000	-0.014142000	-1.393977000
1	3.614922000	0.682464000	-1.513876000
1	3.766836000	-0.823311000	-1.590797000
8	-4.182050000	-0.359675000	-1.545723000
1	-3.524786000	0.360280000	-1.639010000
1	-4.349464000	-0.360739000	-0.586247000
8	2.135087000	-2.440288000	1.208334000
1	1.916478000	-3.307521000	1.570732000
1	1.307505000	-1.882170000	1.358160000
8	2.504721000	-2.195378000	-1.608645000
1	1.640954000	-1.762605000	-1.744460000
1	2.450615000	-2.425609000	-0.659832000
8	-0.122152000	3.275505000	1.612854000
1	0.692466000	2.738999000	1.674408000
1	-0.121522000	3.563410000	0.672520000
8	-1.766369000	1.113075000	1.328591000
1	-1.087074000	0.385715000	1.433356000
1	-1.273442000	1.943766000	1.549585000
8	-4.053822000	-0.276650000	1.403600000
1	-3.298437000	0.357597000	1.490485000
1	-4.678328000	-0.020595000	2.092265000
8	-2.136655000	-2.530784000	1.173220000
1	-2.876811000	-1.929652000	1.368724000
1	-1.339908000	-1.968778000	1.344471000
8	4.130507000	-0.315580000	1.402909000
1	3.637094000	-1.155110000	1.441766000

1	4.319671000	-0.211920000	0.442130000
8	1.816643000	1.582321000	-1.369555000
1	1.246754000	0.842158000	-1.643668000
1	1.825695000	1.480992000	-0.384670000
8	-1.950696000	1.423400000	-1.413266000
1	-1.263791000	0.757171000	-1.613991000
1	-1.956574000	1.371849000	-0.427786000
8	-2.156207000	-2.370217000	-1.630014000
1	-2.190072000	-2.601753000	-0.674762000
1	-2.923192000	-1.765538000	-1.723504000

**15w-V**

8	-0.031261000	-0.658362000	1.648590000
8	2.128072000	-2.377903000	1.226776000
8	-1.852449000	1.268250000	1.395396000
8	-1.806934000	1.413397000	-1.343186000
8	-0.045128000	-0.696599000	-1.199107000
8	0.001662000	3.495273000	-1.569244000
8	1.809643000	1.271455000	1.389703000
8	1.957990000	1.372494000	1.367665000
8	-2.253983000	-2.353456000	1.331619000
8	4.194530000	-0.315576000	1.365192000
8	-2.349309000	-2.553036000	-1.453330000
8	-4.019569000	-0.330441000	-1.444758000
8	-4.264596000	-0.234023000	1.208920000
8	4.202507000	-0.359789000	-1.302036000
8	2.355754000	-2.435663000	-1.541707000
8	-0.029985000	3.471201000	1.281476000
1	-0.015102000	-0.860188000	2.597107000
1	1.532826000	-1.968864000	-1.763172000
1	2.261439000	-2.557452000	-0.567730000
1	-0.708687000	0.025259000	-1.333200000
1	-0.015004000	-0.792993000	-0.223008000
1	0.769722000	2.898870000	-1.670645000
1	-0.007159000	3.649794000	-0.599242000
1	3.563000000	0.364012000	-1.470844000
1	3.650070000	-1.156066000	-1.486397000
1	-1.267097000	2.207673000	-1.571356000
1	-1.860249000	1.453149000	-0.356917000
1	1.329790000	-1.814218000	1.376754000
1	4.295954000	-0.328090000	0.369647000
1	0.731202000	2.885673000	1.455894000
1	-0.785134000	2.877771000	1.455755000
1	-2.729678000	0.870454000	1.547545000
1	-1.191898000	0.524335000	1.545489000
1	-5.191160000	-0.164315000	1.465359000
1	-4.264283000	-0.253563000	0.208480000
1	-2.985833000	-1.724062000	1.459380000
1	-1.445367000	-1.795958000	1.437085000
1	2.668955000	0.856991000	1.591458000
1	1.135312000	0.538538000	1.525269000
1	1.943609000	1.437218000	-0.381665000
1	1.333645000	0.629787000	-1.501272000
1	-2.337195000	-2.645746000	-0.472859000
1	-1.489688000	-2.123687000	-1.611981000
1	-3.370360000	0.376872000	-1.628664000
1	-3.488751000	-1.155261000	-1.558584000
1	2.869217000	-1.781003000	1.433729000
1	5.092350000	-0.292719000	1.715466000

**OH(H<sub>2</sub>O)<sub>16</sub>**

**16w-I**

8	0.238485000	-0.339735000	1.744030000
8	-1.703094000	-2.188888000	1.263651000
8	2.164327000	-2.099296000	1.551968000
8	2.209290000	1.507462000	1.180946000
8	1.804025000	1.635665000	-1.526194000
8	-0.064021000	-0.222826000	-1.045394000
8	-2.422041000	-1.886341000	-1.439278000
8	0.049890000	3.763316000	-1.549843000
8	1.624257000	-2.503047000	-1.168128000
8	-1.593078000	1.788588000	1.502121000
8	4.323943000	-0.280488000	0.943755000
8	-2.094827000	1.816753000	-1.258872000
8	-4.362516000	0.251753000	-1.046571000
8	0.472876000	3.807698000	1.249126000
8	-3.763184000	-0.121630000	1.710848000
8	-0.652888000	-4.181707000	-0.537315000

8	3.723772000	-0.511694000	-1.829864000
1	0.082320000	-0.208695000	2.692624000
1	0.191370000	-3.780853000	-0.828154000
1	-1.300013000	-3.753626000	-1.123749000
1	-0.959048000	-1.556076000	1.454971000
1	-1.472994000	1.068933000	-1.352071000
1	-2.981406000	1.381109000	-1.280629000
1	3.051787000	0.997268000	1.210477000
1	1.519505000	0.841908000	1.434827000
1	1.406495000	-1.438040000	1.697055000
1	3.775100000	-1.021466000	1.260400000
1	4.259143000	-0.365793000	-0.032302000
1	-3.089755000	0.583024000	1.799367000
1	-3.230720000	-0.936511000	1.695569000
1	-3.903694000	-0.551775000	-1.358480000
1	-4.317527000	0.141457000	-0.071700000
1	-0.286162000	3.248594000	1.508959000
1	1.225792000	3.194610000	1.343413000
1	0.172036000	3.924336000	-0.587542000
1	-0.811395000	3.309977000	-1.590450000
1	-1.803481000	1.887213000	0.545803000
1	-0.930356000	1.057963000	1.522077000
1	-2.307985000	-1.919554000	-0.462605000
1	-1.657660000	-1.337967000	-1.688546000
1	3.097293000	-1.258801000	-1.795364000
1	3.149980000	0.264770000	-1.966309000
1	0.993739000	-1.753990000	-1.228827000
1	1.898938000	-2.460563000	-0.225577000
1	0.630508000	0.449110000	-1.295206000
1	-0.050580000	-0.216181000	-0.063163000
1	1.265173000	2.446314000	-1.695836000
1	2.019793000	1.700401000	-0.563011000
1	1.992136000	-2.825754000	2.163724000
1	-1.270054000	-2.995984000	0.920372000

**16w-II**

1	6.301442000	3.801797000	4.493861000
8	5.473054000	4.053975000	4.056243000
8	4.995393000	6.095049000	5.828207000
1	4.454666000	5.695069000	6.548946000
1	5.157358000	5.339693000	5.206097000
8	3.521665000	2.801055000	5.385200000
1	3.564338000	1.875887000	5.080230000
1	4.287321000	3.247485000	4.916782000
8	6.238222000	8.033627000	4.215058000
1	5.398884000	8.391239000	3.887875000
1	5.941900000	7.475213000	4.961651000
8	6.713661000	5.857919000	2.413951000
1	6.255504000	5.216708000	3.018486000
1	6.751951000	6.673710000	2.954567000
8	1.056753000	5.978678000	6.024501000
1	0.909545000	5.257966000	5.383473000
1	1.589767000	6.614135000	5.502904000
8	3.531562000	0.382699000	3.828611000
1	3.373197000	-0.550058000	4.015503000
1	2.728769000	0.690838000	3.320203000
8	3.182738000	4.775905000	7.468879000
1	2.378673000	5.196001000	7.090084000
1	3.246611000	3.940483000	6.970241000
8	2.976401000	7.421998000	4.424556000
1	3.684729000	7.006256000	4.966057000
1	2.948817000	6.825439000	3.653772000
8	3.328723000	5.212847000	2.501143000
1	3.759229000	5.724332000	1.756397000
1	4.085121000	4.862042000	3.013776000
8	5.349722000	2.053954000	2.302006000
1	5.386832000	2.789510000	2.985650000
1	4.962133000	1.301260000	2.783825000
8	5.000264000	4.241795000	-1.149175000
1	5.813025000	3.966609000	-0.673994000
1	4.311394000	3.702507000	-0.717199000
8	7.156776000	3.587906000	0.601072000
1	7.232058000	4.373813000	1.171938000
1	6.722256000	2.925734000	1.168561000
8	4.683469000	6.447000000	0.561753000
1	5.507031000	6.334739000	1.084630000
1	4.776811000	5.782802000	-0.158333000
8	1.340441000	3.827118000	4.038156000
1	2.085571000	3.466915000	4.578403000

1	1.813133000	4.401165000	3.405359000
8	3.219313000	2.898457000	0.765091000
1	4.011828000	2.532400000	1.227835000
1	3.091186000	3.731518000	1.262578000
8	1.485993000	1.443305000	2.461783000
1	1.230132000	2.217914000	3.006360000
1	1.969063000	1.866112000	1.718640000

**16w-III**

8	-0.143886000	-0.303933000	1.708991000
8	-2.015397000	1.486888000	1.083207000
8	-2.232329000	-2.069344000	1.537993000
8	-1.812646000	1.491338000	-1.661523000
8	1.703992000	-2.317683000	1.356447000
8	2.474820000	-1.892295000	-1.298656000
8	0.254058000	-0.386525000	-1.043287000
8	4.262955000	0.208681000	-1.146088000
8	-1.740650000	-2.454447000	-1.119290000
8	1.727995000	1.733186000	1.484110000
8	1.938665000	1.944477000	-1.319390000
8	-0.042224000	3.860149000	-1.487355000
8	3.813488000	-0.217865000	1.629693000
8	-0.327711000	3.783850000	1.326063000
8	-4.354708000	-0.150266000	0.983856000
8	-3.826257000	-0.546645000	-1.617272000
8	0.603631000	-4.127402000	-0.623987000
1	-0.004223000	-0.257881000	2.667867000
1	-3.212156000	-1.311247000	-1.590594000
1	-3.226750000	0.206117000	-1.805825000
1	-4.263732000	-0.299633000	0.002042000
1	-5.301110000	-0.068494000	1.147989000
1	-1.338232000	0.803674000	1.374299000
1	-2.882189000	1.069036000	1.240422000
1	1.331377000	1.182842000	-1.392496000
1	1.346930000	2.718823000	-1.481709000
1	0.984560000	-1.649405000	1.502235000
1	-3.025722000	-1.505618000	1.552116000
1	-1.480313000	-1.435012000	1.676200000
1	0.445589000	3.225225000	1.542047000
1	-1.062723000	3.143572000	1.379712000
1	-0.747984000	3.227935000	-1.719602000
1	-0.162960000	3.970234000	-0.517278000
1	3.152554000	0.497242000	1.743960000
1	3.277371000	-1.028185000	1.681255000
1	4.254386000	0.119473000	-0.168196000
1	3.669942000	0.964749000	-1.308286000
1	1.879661000	1.863426000	0.521618000
1	1.036356000	1.023288000	1.518610000
1	-1.912905000	1.558599000	-0.679442000
1	-1.070045000	0.862482000	-1.730826000
1	-0.258745000	-3.733523000	-0.864233000
1	1.223943000	-3.693662000	-1.231878000
1	-1.082151000	-1.735205000	-1.210231000
1	-1.958619000	-2.411555000	-0.152426000
1	1.050569000	-0.954743000	-1.227405000
1	0.203516000	-0.347057000	-0.061253000
1	3.193100000	-1.222355000	-1.397192000
1	2.423985000	-2.031234000	-0.326962000
1	1.246361000	-3.089230000	0.967407000

**16w-IV**

1	0.065933000	-0.274282000	2.663428000
8	0.186462000	-0.416110000	1.711049000
8	2.177152000	-2.110219000	1.531434000
1	1.392801000	-1.479536000	1.662491000
1	1.996166000	-2.865444000	2.104679000
8	0.328187000	3.725233000	1.427715000
1	0.267278000	3.953834000	0.474276000
1	1.098363000	3.125747000	1.454650000
8	-0.576360000	-4.065418000	-0.685155000
1	-1.226498000	-3.646011000	-1.272417000
1	0.269089000	-3.655585000	-0.958721000
8	-1.697486000	-2.347873000	1.356970000
1	-0.973655000	-1.680119000	1.501422000
1	-1.251668000	-3.090607000	0.902326000
8	3.897397000	-0.433384000	-1.752616000
1	3.290504000	0.323878000	-1.870951000
1	3.290604000	-1.197744000	-1.752649000
8	0.077794000	3.958780000	-1.396775000

1	0.756549000	3.296618000	-1.632474000
1	-0.747579000	3.443585000	-1.480907000
8	4.298672000	-0.199795000	1.048609000
1	3.767447000	-0.965554000	1.333992000
1	4.306595000	-0.293410000	0.070546000
8	1.760052000	-2.408094000	-1.222557000
1	1.991106000	-2.397937000	-0.267612000
1	1.109900000	-1.676060000	-1.284564000
8	-0.218541000	-0.377471000	-1.094177000
1	-1.032652000	-0.924843000	-1.256841000
1	-0.169876000	-0.310763000	-0.116275000
8	-1.566460000	1.723066000	1.444512000
1	-0.926121000	0.971970000	1.497707000
1	-0.988522000	2.516003000	1.568733000
8	-4.333964000	0.162840000	-1.160440000
1	-4.309745000	0.088843000	-0.182871000
1	-3.712535000	0.898887000	-1.326397000
8	-3.745791000	-0.155239000	1.620715000
1	-3.197080000	-0.956268000	1.680503000
1	-3.108907000	0.574764000	1.739177000
8	-2.470632000	-1.865857000	-1.298259000
1	-2.421591000	-2.005736000	-0.327413000
1	-3.215985000	-1.225397000	-1.398837000
8	2.082570000	1.481452000	1.112265000
1	2.947112000	1.016036000	1.197066000
1	1.418066000	0.790107000	1.365975000
8	-2.046787000	1.954647000	-1.263056000
1	-1.962279000	1.934458000	-0.278255000
1	-1.426691000	1.242428000	-1.502473000
8	1.808317000	1.608541000	-1.623876000
1	1.934473000	1.624960000	-0.642397000
1	1.084747000	0.962382000	-1.715776000

#### 16w-V

8	-0.167477000	-0.302656000	1.706554000
8	-2.036497000	1.499934000	1.084623000
8	-2.254521000	-2.073427000	1.520934000
8	1.704692000	-2.271196000	1.403979000
8	2.499944000	-1.912818000	-1.247667000
8	0.248064000	-0.431567000	-1.077246000
8	4.352885000	0.138198000	-1.124348000
8	-1.786416000	1.479415000	-1.660241000
8	-1.725982000	-2.502973000	-1.125630000
8	1.578414000	1.787692000	1.422878000
8	-0.337951000	3.807816000	1.317055000
8	2.046915000	1.908009000	-1.282752000
8	3.744413000	-0.099499000	1.654189000
8	-0.073393000	3.877085000	-1.524203000
8	-3.787630000	-0.569938000	-1.651510000
8	-4.365510000	-0.152892000	0.934235000
8	0.638158000	-4.139972000	-0.546310000
1	-0.053423000	-0.257963000	2.668975000
1	-3.178392000	-1.338072000	-1.616225000
1	-3.183247000	0.181845000	-1.828456000
1	-4.255540000	-0.311302000	-0.044367000
1	-5.315410000	-0.078112000	1.080574000
1	-1.366222000	0.809813000	1.370855000
1	-2.905866000	1.079593000	1.219990000
1	1.966350000	1.924994000	-0.296285000
1	1.442401000	1.172203000	-1.490518000
1	0.967467000	-1.615213000	1.525282000
1	-3.047206000	-1.508470000	1.519848000
1	-1.503868000	-1.437969000	1.657978000
1	-0.270167000	3.978615000	0.352554000
1	-1.082343000	3.179076000	1.368493000
1	0.752326000	3.355437000	-1.568329000
1	-0.748029000	3.206215000	-1.741861000
1	3.109723000	0.635624000	1.751299000
1	3.190444000	-0.896398000	1.725791000
1	4.315629000	0.087112000	-0.145277000
1	3.727080000	0.864214000	-1.314707000
1	1.013772000	2.589178000	1.526543000
1	0.927797000	1.040723000	1.507881000
1	-1.899533000	1.556698000	-0.680604000
1	-1.042506000	0.850022000	-1.718030000
1	-0.225646000	-3.763773000	-0.807978000
1	1.261811000	-3.712228000	-1.155194000
1	-1.957257000	-2.445176000	-0.163169000
1	-1.064625000	-1.785963000	-1.219082000

1	1.063699000	-0.979201000	-1.234055000
1	0.197681000	-0.352604000	-0.099250000
1	3.243494000	-1.271507000	-1.349014000
1	2.427499000	-2.024024000	-0.273310000
1	1.267245000	-3.063076000	1.033318000

#### OH(H<sub>2</sub>O)<sub>17</sub>

##### 17w-I

1	-0.008274000	0.014845000	2.667663000
8	0.073738000	0.042828000	1.701638000
8	3.964762000	-0.366974000	-1.479748000
1	3.442929000	0.451183000	-1.627121000
1	3.300992000	-1.069210000	-1.644466000
8	4.176308000	-0.331568000	1.194494000
1	4.194918000	-0.356144000	0.196824000
1	5.093663000	-0.443654000	1.470228000
8	1.786594000	-1.935333000	1.212845000
1	1.151354000	-1.188196000	1.432056000
1	2.666501000	-1.559040000	1.398573000
8	-2.162282000	-1.955427000	-1.370443000
1	-1.441522000	-1.297631000	-1.429442000
1	-1.687543000	-2.814183000	-1.475936000
8	-1.624488000	2.175406000	1.369099000
1	-1.023629000	2.951496000	1.451349000
1	-1.012420000	1.406484000	1.507880000
8	2.135099000	1.733624000	1.308350000
1	2.927329000	1.191455000	1.475534000
1	1.374087000	1.110494000	1.494719000
8	0.392143000	4.092901000	1.223504000
1	1.140973000	3.486506000	1.364435000
1	0.344500000	4.171644000	0.245651000
8	-0.260059000	-3.966230000	1.460013000
1	-0.957954000	-3.296308000	1.609652000
1	0.558448000	-3.441561000	1.533081000
8	-0.468059000	-4.153154000	-1.356713000
1	0.342334000	-3.661614000	-1.585575000
1	-0.399795000	-4.228810000	-0.378627000
8	-3.970361000	0.461220000	1.449721000
1	-3.419209000	-0.331696000	1.612348000
1	-3.338973000	1.193240000	1.574613000
8	-4.102524000	0.245217000	-1.363065000
1	-4.198402000	0.293355000	-0.385339000
1	-3.669939000	-0.615853000	-1.503215000
8	-2.073515000	-1.706722000	1.438402000
1	-2.194724000	-1.833080000	0.470773000
1	-1.306343000	-1.083194000	1.498226000
8	1.684888000	-2.114940000	-1.530157000
1	1.730546000	-2.125317000	-0.541768000
1	1.039442000	-1.401405000	-1.684092000
8	0.171288000	3.957414000	-1.608590000
1	0.885829000	3.306317000	-1.747398000
1	-0.639634000	3.431227000	-1.733169000
8	2.086893000	1.761698000	-1.463710000
1	1.333689000	1.135489000	-1.507022000
1	2.170596000	1.866345000	-0.485508000
8	-0.162055000	0.074937000	-1.098360000
1	-0.828891000	0.798974000	-1.270848000
1	-0.102873000	0.047939000	-0.118760000
8	-1.984336000	2.015846000	-1.341086000
1	-2.806794000	1.490463000	-1.493707000
1	-1.973458000	2.153485000	-0.361164000

##### 17w-II

1	-0.002842000	0.018535000	2.660210000
8	-0.066375000	-0.040612000	1.694266000
8	-3.805568000	-1.136429000	-1.593465000
1	-4.027532000	-1.194886000	-0.645381000
1	-3.034352000	-1.735562000	-1.672505000
8	-3.934620000	-1.086424000	1.324625000
1	-4.687029000	-0.985686000	1.919781000
1	-3.454141000	-0.212333000	1.355648000
8	-2.421765000	1.117795000	1.186768000
1	-2.408555000	1.238596000	0.209789000
1	-1.529597000	0.703140000	1.391163000
8	1.241452000	2.606816000	-1.404790000
1	0.457161000	3.195750000	-1.509548000
1	0.847226000	1.713363000	-1.447050000
8	2.320348000	-1.381586000	1.389413000

1	2.053329000	-2.325359000	1.483559000
1	1.464857000	-0.897156000	1.520197000
8	-1.333348000	-2.394537000	1.320604000
1	-2.267084000	-2.190275000	1.508264000
1	-0.865373000	-1.527181000	1.495364000
8	1.174353000	-3.915051000	1.279730000
1	0.250592000	-3.635922000	1.410988000
1	1.252171000	-3.990327000	0.303463000
8	-1.252393000	3.780255000	1.463591000
1	-0.341285000	3.447383000	1.594801000
1	-1.784976000	2.965901000	1.544032000
8	-1.201943000	3.927084000	-1.363988000
1	-1.784519000	3.180821000	-1.589068000
1	-1.283437000	3.990274000	-0.386041000
8	3.852484000	1.089564000	1.427400000
1	3.041927000	1.616661000	1.584045000
1	3.546126000	0.175009000	1.567597000
8	3.882294000	1.303248000	-1.385358000
1	3.990764000	1.308665000	-0.407579000
1	3.159937000	1.938431000	-1.534808000
8	1.284335000	2.379319000	1.406600000
1	1.337896000	2.533191000	0.436805000
1	0.799736000	1.518641000	1.478623000
8	-2.314321000	1.214158000	-1.616413000
1	-2.933910000	0.457047000	-1.740997000
1	-1.434868000	0.796808000	-1.674924000
8	1.339478000	-3.763383000	-1.553521000
1	0.432578000	-3.432947000	-1.703513000
1	1.892792000	-2.973453000	-1.692915000
8	-1.262223000	-2.452660000	-1.453160000
1	-1.317805000	-2.568684000	-0.474727000
1	-0.799298000	-1.590784000	-1.497985000
8	0.191807000	-0.033920000	-1.081009000
1	1.079684000	-0.456245000	-1.261578000
1	0.135560000	-0.025806000	-0.100366000
8	2.606383000	-1.144751000	-1.327313000
1	3.164498000	-0.346534000	-1.491667000
1	2.646742000	-1.260170000	-0.345518000

**17w-III**

1	-0.029123000	-0.016749000	2.651721000
8	-0.099407000	-0.042590000	1.684645000
8	-3.944159000	0.255525000	-1.516588000
1	-3.406690000	-0.553950000	-1.655794000
1	-3.292405000	0.970218000	-1.675188000
8	-4.191077000	0.242288000	1.154751000
1	-4.196066000	0.255390000	0.156726000
1	-5.114920000	0.334772000	1.415814000
8	-1.844399000	1.915481000	1.204091000
1	-1.197916000	1.178551000	1.419710000
1	-2.717757000	1.516999000	1.374351000
8	2.215161000	1.952652000	-1.337760000
1	2.219040000	1.962908000	-0.349527000
1	1.503186000	1.304677000	-1.499162000
8	1.671395000	-2.098746000	1.405082000
1	1.105019000	-2.898526000	1.501515000
1	1.020569000	-1.355867000	1.515919000
8	-2.114053000	-1.787296000	1.295073000
1	-2.919774000	-1.262509000	1.452669000
1	-1.370494000	-1.141455000	1.474082000
8	-0.281617000	-4.085510000	1.281038000
1	-1.052007000	-3.503140000	1.405929000
1	-0.226402000	-4.180466000	0.304939000
8	0.161810000	4.009368000	1.443405000
1	0.214879000	4.207099000	0.482555000
1	-0.655498000	3.482795000	1.510255000
8	0.345349000	4.175011000	-1.388626000
1	1.087845000	3.547705000	-1.498246000
1	-0.427527000	3.620883000	-1.606584000
8	3.919202000	-0.263253000	1.477998000
1	3.382229000	0.537431000	1.625624000
1	3.288421000	-0.992033000	1.625479000
8	4.174604000	-0.236781000	-1.346188000
1	4.245337000	-0.244989000	-0.366218000
1	3.681438000	0.590411000	-1.507562000
8	1.905049000	1.826262000	1.408965000
1	1.421059000	2.671633000	1.556486000
1	1.185581000	1.149167000	1.495834000
8	-1.706970000	2.059381000	-1.539572000

1	-1.765305000	2.078876000	-0.551924000
1	-1.046541000	1.356646000	-1.682496000
8	-0.053167000	-3.994880000	-1.551442000
1	-0.784913000	-3.368478000	-1.712086000
1	0.743867000	-3.447973000	-1.677843000
8	-2.036751000	-1.849551000	-1.476605000
1	-2.128872000	-1.944526000	-0.498301000
1	-1.295429000	-1.208733000	-1.520580000
8	0.163398000	-0.103595000	-1.137295000
1	0.859457000	-0.804447000	-1.285191000
1	0.106357000	-0.047134000	-0.159482000
8	2.048087000	-1.998697000	-1.303996000
1	2.877271000	-1.484036000	-1.458280000
1	2.026430000	-2.111719000	-0.320951000

**17w-IV**

1	-0.007538000	0.049573000	2.675596000
8	0.070525000	0.048769000	1.709030000
8	3.858170000	-1.179693000	-1.558681000
1	3.065970000	-1.746900000	-1.652671000
1	4.044203000	-1.208992000	-0.601827000
8	3.945476000	-0.968428000	1.360300000
1	4.686740000	-0.897106000	1.973169000
1	3.476963000	-0.089062000	1.406573000
8	1.361715000	-2.237896000	1.235198000
1	0.885101000	-1.379759000	1.447982000
1	2.292760000	-2.041014000	1.444483000
8	-2.490364000	-1.500581000	-1.359202000
1	-1.652752000	-0.999551000	-1.413411000
1	-2.195720000	-2.437165000	-1.461027000
8	-1.187408000	2.471862000	1.351767000
1	-0.449593000	3.118888000	1.435790000
1	-0.735808000	1.601053000	1.501016000
8	2.447822000	1.257872000	1.247793000
1	2.467155000	1.334810000	0.265502000
1	1.556868000	0.843872000	1.438763000
8	1.173606000	3.948787000	1.225509000
1	1.755419000	3.183776000	1.389835000
1	1.167270000	4.006526000	0.245193000
8	-1.045869000	-3.825018000	1.485827000
1	-1.597863000	-3.029883000	1.630777000
1	-0.139831000	-3.472637000	1.559106000
8	-1.272450000	-3.990825000	-1.331483000
1	-0.379112000	-3.672923000	-1.559160000
1	-1.224988000	-4.071341000	-0.352649000
8	-3.820612000	1.246448000	1.404350000
1	-3.436885000	0.363753000	1.584324000
1	-3.061676000	1.843609000	1.536181000
8	-3.943145000	1.042952000	-1.409901000
1	-4.044553000	1.116144000	-0.434271000
1	-3.690327000	0.111249000	-1.538143000
8	-2.380841000	-1.250703000	1.448662000
1	-2.514091000	-1.360005000	0.480426000
1	-1.507353000	-0.789061000	1.513579000
8	1.240277000	-2.422090000	-1.508155000
1	1.282518000	-2.432376000	-0.520150000
1	0.751974000	-1.595212000	-1.669150000
8	1.017086000	3.757591000	-1.609368000
1	1.606833000	3.004456000	-1.792499000
1	0.124215000	3.396799000	-1.759803000
8	2.391212000	1.195900000	-1.547352000
1	3.020957000	0.454514000	-1.697636000
1	1.520592000	0.745202000	-1.504404000
8	-0.139648000	0.102641000	-1.066434000
1	-0.643976000	0.944164000	-1.257464000
1	-0.106815000	0.070974000	-0.085322000
8	-1.523401000	2.366602000	-1.366553000
1	-2.429663000	2.008862000	-1.531100000
1	-1.504194000	2.511243000	-0.388051000

**17w-V**

1	-0.001711000	0.033347000	2.650935000
8	0.105954000	0.026778000	1.686967000
8	-0.509397000	4.048321000	-1.483522000
1	0.340308000	3.609116000	-1.675506000
1	-0.451304000	4.184037000	-0.511071000
8	-0.287145000	4.024882000	1.334430000
1	-0.958668000	3.325373000	1.479848000
1	0.551806000	3.550242000	1.472265000

8	1.865468000	2.028284000	1.303676000	1	4.526500000	1.687724000	-0.556556000
1	2.734264000	1.615879000	1.459019000	1	-3.603929000	-2.909274000	-1.140145000
1	1.215456000	1.285719000	1.474152000	1	-4.388854000	-1.789435000	-0.437965000
8	1.986505000	-1.902105000	-1.368648000	1	0.956112000	2.833683000	-1.497986000
1	1.472306000	-2.721448000	-1.578562000	1	0.154750000	1.725890000	-0.746225000
1	2.094715000	-1.941037000	-0.386708000	1	1.184562000	0.021054000	2.183747000
8	-1.743966000	-2.001351000	1.346081000	1	1.109445000	-0.002954000	0.628199000
1	-2.599984000	-1.555883000	1.554592000	1	-3.563702000	3.110240000	0.322277000
1	-1.080983000	-1.273909000	1.464855000	1	-3.498566000	2.931205000	-1.189335000
8	-2.025877000	1.755145000	1.338599000	1	3.092300000	2.769295000	-2.010900000
1	-2.154350000	1.788906000	0.365191000	1	2.253174000	1.737199000	-2.760035000
1	-1.264725000	1.129341000	1.445149000	1	4.263676000	-1.219719000	-0.335519000
8	-3.980187000	-0.379342000	1.592593000	1	3.460751000	-0.183674000	0.469054000
1	-3.453457000	0.439369000	1.685048000	1	-0.916872000	-2.891364000	3.078207000
1	-4.219012000	-0.356161000	0.640866000	1	0.611379000	-2.951990000	3.011790000
8	4.194375000	0.293818000	1.163582000	1	-3.008425000	-0.056733000	-1.790640000
1	5.132298000	0.356784000	1.379347000	1	-1.065526000	3.204804000	0.565406000
1	4.155430000	0.269888000	0.167559000	1	-1.114702000	3.185890000	2.106139000
8	3.852323000	0.240316000	-1.502330000	1	1.211175000	-3.093351000	-1.705616000
1	3.214429000	0.972570000	-1.644249000	1	1.987235000	-2.043175000	-2.494386000
1	3.325928000	-0.562933000	-1.682184000	1	-4.300358000	1.063717000	-0.384265000
8	0.314225000	-3.991733000	1.278017000	1	-3.339952000	0.121046000	0.326554000
1	1.034830000	-3.366205000	1.473513000	1	-1.869828000	1.338431000	1.367151000
1	-0.490176000	-3.468269000	1.459578000	1	-1.128745000	0.225487000	0.557811000
8	0.257971000	-4.022886000	-1.554536000	1	3.531234000	-3.188700000	-0.333299000
1	0.272620000	-4.170451000	-0.582926000	1	3.461380000	-3.122894000	-1.181499000
1	-0.580433000	-3.536146000	-1.676264000	1	-2.162833000	1.862513000	-2.727157000
8	2.116350000	-1.694193000	1.362490000	1	-1.322479000	2.890397000	-1.968393000
1	2.929307000	-1.177172000	1.509121000	1	2.847470000	-0.167456000	-1.661577000
1	1.374915000	-1.036905000	1.525922000	1	1.303570000	-0.090329000	-1.721066000
8	1.764877000	2.180035000	-1.468145000	1	-2.229572000	-1.485161000	1.678143000
1	1.852213000	2.262760000	-0.488465000	1	-2.978432000	-2.661873000	1.023055000
1	1.102558000	1.459939000	-1.519283000	1	0.960219000	3.040256000	2.818852000
8	-4.209993000	-0.266095000	-1.250384000	1	0.159628000	2.066994000	3.690802000
1	-3.715725000	0.547941000	-1.453561000	1	1.495910000	2.932182000	0.589394000
1	-3.562142000	-0.970170000	-1.451062000	1	2.160912000	1.829202000	1.386730000
8	-2.117475000	1.796990000	-1.496143000	1	-1.318191000	-2.903577000	-1.727345000
1	-1.652442000	2.663294000	-1.598733000	1	-0.145257000	-1.581701000	-0.473696000
1	-1.399222000	1.148740000	-1.606914000	1	-0.917379000	-2.652872000	0.359654000
8	0.043746000	-0.048266000	-1.116461000	1	-2.253781000	-1.019979000	-2.736231000
1	0.755915000	-0.720918000	-1.292609000	1	-1.743913000	-3.567210000	-3.064480000
1	0.000258000	-0.017619000	-0.136070000				
8	-1.964437000	-2.114195000	-1.410963000				
1	-1.947316000	-2.183256000	-0.425112000				
1	-1.334249000	-1.380007000	-1.540110000				

### OH(H<sub>2</sub>O)<sub>23</sub>

#### 23w-I

8	-0.096476000	0.021597000	-0.661042000
8	-1.791831000	0.352251000	1.315817000
8	-0.243889000	-2.586188000	-0.359438000
8	0.249010000	2.717149000	-0.806878000
8	2.297614000	2.698097000	-2.583948000
8	-1.687825000	3.089625000	1.309251000
8	0.163016000	2.991058000	3.384853000
8	2.102433000	-0.183936000	-2.301731000
8	-4.064833000	0.105289000	-0.334152000
8	-2.311394000	-0.080137000	-2.486036000
8	-4.122934000	2.856310000	-0.431505000
8	-2.174838000	2.791631000	-2.434821000
8	-2.204971000	-2.457933000	1.602079000
8	-4.143841000	-2.730847000	-0.348837000
8	-0.004276000	0.040586000	3.427846000
8	1.756147000	-0.013596000	1.371065000
8	-0.122553000	-2.731592000	3.619309000
8	-2.046794000	-2.940537000	-2.395423000
8	4.356292000	2.643576000	-0.637391000
8	1.890084000	-2.887431000	1.514115000
8	2.155205000	2.805403000	1.307093000
8	4.088168000	-0.249733000	-0.272848000
8	4.096987000	-3.014312000	-0.441489000
8	1.951663000	-3.011416000	-2.328616000
1	-0.780020000	0.036868000	-1.366780000
1	-0.044606000	-0.908312000	3.692986000
1	-0.749476000	0.128806000	2.791366000
1	1.212107000	-2.964799000	0.809819000
1	2.006474000	-1.916285000	1.545966000
1	3.774108000	2.830631000	0.123213000

#### 23w-II

8	-0.114582000	0.019308000	-0.677596000
8	-1.819225000	0.023246000	1.319511000
8	0.135727000	-2.674060000	-0.596543000
8	-0.075464000	2.671019000	-0.655078000
8	1.984964000	3.065884000	-2.331405000
8	-1.914691000	2.778191000	1.555344000
8	-0.112747000	2.598198000	3.650056000
8	2.100720000	0.216604000	-2.296711000
8	-4.133557000	-0.192872000	-0.290098000
8	-2.388275000	-0.002929000	-2.461366000
8	-4.278188000	2.611306000	-0.158636000
8	-2.283848000	2.876400000	-2.251594000
8	-1.915562000	-2.857776000	1.308641000
8	-3.911672000	-3.088298000	-0.545755000
8	-0.020044000	-0.338671000	3.413551000
8	1.722474000	-0.003992000	1.371162000
8	0.148247000	-3.098820000	3.327901000
8	-2.019630000	-2.831685000	-2.615647000
8	4.038484000	3.075143000	-0.398265000
8	2.221893000	-2.870611000	1.292400000
8	1.834559000	2.804334000	1.526273000
8	4.068600000	0.166694000	-0.259857000
8	4.442503000	-2.532649000	-0.623735000
8	2.403558000	-2.614370000	-2.571908000
1	-0.809969000	-0.043160000	-1.368001000
1	0.039303000	-1.310675000	3.578345000
1	-0.771494000	-0.262877000	2.783365000
1	1.566922000	-2.953181000	0.563217000
1	2.233129000	-1.901598000	1.414138000
1	3.448336000	3.127158000	0.376976000
1	4.309340000	2.138390000	-0.401409000
1	-3.337968000	-3.065161000	-1.344651000
1	-4.302181000	-2.196916000	-0.525242000
1	0.666192000	2.915441000	-1.279308000
1	-0.056082000	1.660068000	-0.655292000
1	1.155297000	-0.119164000	2.179865000

1	1.078844000	-0.040841000	0.626389000
1	-3.680888000	2.803313000	0.586687000
1	-3.725163000	2.826759000	-0.933056000
1	2.769138000	3.189086000	-1.750700000
1	2.056143000	2.117772000	-2.572390000
1	4.366504000	-0.768262000	-0.390324000
1	3.435990000	0.095683000	0.477133000
1	-0.615039000	-3.286965000	2.750870000
1	0.914101000	-3.194053000	2.726876000
1	-3.078255000	-0.082775000	-1.763395000
1	-1.274713000	2.967881000	0.842483000
1	-1.372291000	2.826307000	2.378778000
1	1.618994000	-2.902619000	-2.076971000
1	2.263779000	-1.648644000	-2.665048000
1	-4.412467000	0.748188000	-0.241155000
1	-3.394774000	-0.214539000	0.354492000
1	-1.967108000	0.988730000	1.463240000
1	-1.153279000	0.013288000	0.553062000
1	3.902013000	-2.853622000	0.121663000
1	3.827546000	-2.651344000	-1.381911000
1	-1.458117000	2.887928000	-1.702542000
1	2.833122000	0.231472000	-1.641068000
1	1.290075000	0.141577000	-1.729500000
1	-2.019584000	-1.904363000	1.480419000
1	-2.695334000	-3.063071000	0.732550000
1	0.671786000	2.771335000	3.091645000
1	-0.037261000	1.650204000	3.860695000
1	1.169330000	2.939625000	0.820696000
1	1.922537000	1.826471000	1.515267000
1	-2.077668000	-1.885493000	-2.842916000
1	-1.195695000	-2.885791000	-2.097069000
1	0.098478000	-1.675949000	-0.637266000
1	-0.576133000	-2.873793000	0.054622000
1	-2.385033000	0.948309000	-2.672098000
1	-2.154364000	3.573118000	-2.907305000

**23w-III**

1	-0.826315000	0.038936000	-1.341010000
8	-0.125337000	-0.042204000	-0.658628000
8	0.217313000	0.260605000	3.437103000
1	0.285667000	1.231389000	3.603632000
1	0.903298000	0.105313000	2.753498000
8	-1.739701000	3.049807000	1.383352000
1	-1.091553000	3.061992000	0.643349000
1	-1.868317000	2.086100000	1.496562000
8	-4.324984000	-2.467128000	-0.300674000
1	-3.728729000	-2.616807000	0.462889000
1	-4.487464000	-1.504162000	-0.265829000
8	4.305038000	2.599120000	-0.647459000
1	3.716878000	2.688051000	-1.431687000
1	4.564670000	1.660396000	-0.670065000
8	-0.331373000	-2.697579000	-0.621156000
1	-1.030668000	-2.884188000	-1.282472000
1	-0.235485000	-1.692227000	-0.649132000
8	-1.687397000	0.169287000	1.466030000
1	-1.083089000	0.205649000	2.248683000
1	-1.067715000	0.103264000	0.665301000
8	4.043943000	-3.063824000	-0.350116000
1	3.488767000	-3.216708000	0.432697000
1	3.401362000	-3.167136000	-1.088505000
8	-2.594157000	-2.836522000	-2.311178000
1	-3.311278000	-2.774692000	-1.621093000
1	-2.876133000	-3.526398000	-2.923834000
8	-4.010678000	0.357608000	-0.126565000
1	-4.185797000	1.327415000	-0.235013000
1	-3.333105000	0.330811000	0.576037000
8	0.395447000	3.021972000	3.356519000
1	1.160342000	3.127007000	2.761275000
1	-0.370101000	3.206075000	2.775545000
8	2.077120000	-0.182896000	-2.391072000
1	1.293948000	-0.121205000	-1.789080000
1	2.845490000	-0.195153000	-1.778136000
8	1.641421000	-2.981270000	1.463203000
1	0.990538000	-3.150628000	0.756291000
1	1.099526000	-2.987242000	2.288595000
8	-2.028757000	2.885651000	-2.453329000
1	-1.190341000	2.990589000	-1.972955000
1	-2.053360000	1.937540000	-2.678598000
8	4.149029000	-0.286312000	-0.458329000

1	4.320702000	-1.256929000	-0.444345000
1	3.460111000	-0.199480000	0.229489000
8	1.828554000	-0.281384000	1.194065000
1	1.856148000	-1.266008000	1.316307000
1	1.146991000	-0.167933000	0.489568000
8	-4.019868000	3.069159000	-0.451752000
1	-3.417858000	3.105079000	-1.227421000
1	-3.409976000	3.286382000	0.278967000
8	2.041838000	-3.040881000	-2.316881000
1	2.071611000	-2.091217000	-2.557721000
1	1.223165000	-3.087442000	-1.789460000
8	-2.403001000	0.048164000	-2.383058000
1	-2.459754000	-0.881994000	-2.664963000
1	-3.033191000	0.109563000	-1.628749000
8	2.374137000	2.566433000	1.273950000
1	2.357205000	1.605204000	1.426118000
1	3.151074000	2.682093000	0.667003000
8	-0.093404000	-2.650839000	3.599334000
1	-0.922028000	-2.717136000	3.084604000
1	-0.041182000	-1.705542000	3.829592000
8	-2.163136000	-2.570241000	1.564569000
1	-1.517125000	-2.770202000	0.852756000
1	-2.106783000	-1.587057000	1.595165000
8	2.350851000	2.653982000	-2.674767000
1	2.259474000	1.688563000	-2.811952000
1	1.571214000	2.849866000	-2.124548000
8	0.261526000	2.638496000	-0.558469000
1	0.147376000	1.645831000	-0.601132000
1	1.016398000	2.740751000	0.066253000

**23w-IV**

8	-0.114749000	-0.003518000	-0.691991000
8	-1.806586000	0.184452000	1.278363000
8	-0.103538000	-2.657189000	-0.601407000
8	0.225814000	2.707798000	-0.656918000
8	2.282856000	2.877164000	-2.404520000
8	-1.670090000	2.913078000	1.462433000
8	0.123185000	2.718058000	3.562905000
8	2.125787000	-0.007837000	-2.308753000
8	-4.159313000	0.043374000	-0.201657000
8	-2.413248000	0.245618000	-2.428378000
8	-4.039265000	2.986372000	-0.203961000
8	-2.170857000	2.985113000	-2.368715000
8	-2.135341000	-2.640220000	1.397507000
8	-4.143164000	-2.800202000	-0.570702000
8	-0.030510000	-0.229352000	3.403208000
8	1.734349000	-0.104366000	1.344627000
8	-0.037668000	-3.006982000	3.391900000
8	-2.306206000	-2.533010000	-2.479066000
8	4.331708000	2.742515000	-0.447797000
8	1.971391000	-2.975808000	1.309794000
8	2.105070000	2.708952000	1.479626000
8	4.096726000	-0.158458000	-0.269434000
8	4.237185000	-2.895095000	-0.590530000
8	2.194745000	-2.838326000	-2.539567000
1	-0.811865000	0.065002000	-1.380825000
1	-0.032321000	-1.196767000	3.595996000
1	-0.773671000	-0.123312000	2.768863000
1	1.325390000	-3.033125000	0.572061000
1	2.057225000	-2.005262000	1.396962000
1	3.740376000	2.868630000	0.317881000
1	4.511857000	1.784835000	-0.429155000
1	-3.505445000	-2.752692000	-1.340907000
1	0.938147000	2.888730000	-1.329865000
1	0.132275000	1.715388000	-0.680282000
1	1.160585000	-0.136594000	2.154422000
1	1.089849000	-0.066716000	0.600312000
1	-3.414343000	3.059226000	0.539872000
1	3.072588000	2.928287000	-1.822696000
1	2.257942000	1.928053000	-2.640979000
1	4.314365000	-1.116032000	-0.385137000
1	3.458463000	-0.162150000	0.465697000
1	-0.827417000	-3.147861000	2.840145000
1	0.701278000	-3.158354000	2.767336000
1	-3.097145000	0.233506000	-1.726474000
1	-1.031359000	3.070934000	0.738843000
1	-1.121178000	2.969962000	2.280696000
1	1.387535000	-3.045176000	-2.041029000
1	2.145066000	-1.863182000	-2.640974000



1	-3.384321000	0.016443000	0.402771000
1	-1.859352000	1.165028000	1.408008000
1	-1.135880000	0.103051000	0.511339000
1	3.668327000	-3.145260000	0.160712000
1	3.613965000	-2.972682000	-1.346765000
1	-1.340389000	3.058766000	-1.862241000
1	2.854745000	-0.019755000	-1.650225000
1	1.309040000	0.005942000	-1.747699000
1	-2.165784000	-1.670367000	1.506551000
1	-2.931820000	-2.843038000	0.866170000
1	0.919678000	2.815282000	3.001193000
1	0.128102000	1.774348000	3.801756000
1	1.455213000	2.868011000	0.759676000
1	2.129867000	1.729680000	1.489382000
1	-2.283247000	-1.581616000	-2.712240000
1	-1.459227000	-2.676545000	-2.011943000
1	-0.058024000	-1.649169000	-0.643970000
1	-0.793328000	-2.799226000	0.081868000
1	-2.310872000	1.208620000	-2.618452000
1	-2.862602000	3.110934000	-1.685372000
1	-4.330606000	2.058772000	-0.176883000
1	-4.435519000	-0.888156000	-0.281584000
1	-4.792397000	-3.471444000	-0.812368000

**23w-V**

1	-0.821748000	-0.048255000	-1.315699000
8	-0.132925000	-0.020552000	-0.616075000
8	0.103529000	-0.057395000	3.468549000
1	0.068579000	0.895490000	3.716991000
1	0.812112000	-0.083916000	2.790615000
8	-2.138264000	2.670288000	1.585589000
1	-1.445292000	2.777848000	0.895354000
1	-2.170505000	1.692420000	1.651383000
8	-4.059024000	-2.948283000	-0.618391000
1	-3.460199000	-3.094832000	0.139488000
1	-4.328622000	-2.018718000	-0.512400000
8	3.877685000	3.081689000	-0.428798000
1	3.290098000	3.169125000	-1.210742000
1	4.242066000	2.181509000	-0.518535000
8	0.031947000	-2.743798000	-0.810196000
1	-0.666422000	-2.904929000	-1.499157000
1	0.020233000	-1.750689000	-0.728816000
8	-1.773181000	-0.159484000	1.464392000
1	-1.188761000	-0.149275000	2.262245000
1	-1.130824000	-0.099639000	0.683850000
8	4.388024000	-2.532228000	-0.496802000
1	3.861603000	-2.828439000	0.264474000
1	3.765448000	-2.664713000	-1.249100000
8	-2.034245000	-2.853360000	-2.571953000
1	-2.817805000	-2.953764000	-1.986256000
1	-2.085181000	-1.919111000	-2.841613000
8	-4.057932000	-0.047200000	-0.211941000
1	-4.311308000	0.903321000	-0.254040000
1	-3.409424000	-0.079514000	0.516892000
8	-0.016100000	2.724366000	3.611146000
1	0.731946000	2.958247000	3.032085000
1	-0.798100000	2.874610000	3.044798000
8	2.051556000	0.231017000	-2.360148000
1	1.272480000	0.134100000	-1.757814000
1	2.817250000	0.250535000	-1.743842000
8	1.982446000	-2.934012000	1.283492000
1	1.373454000	-3.128888000	0.544769000
1	1.427247000	-3.082289000	2.086122000
8	-1.972739000	2.940745000	-2.273271000
1	-1.244134000	2.977067000	-1.617097000
1	-1.660154000	3.483324000	-3.008805000
8	4.098302000	0.216661000	-0.403751000
1	4.405925000	-0.719559000	-0.461522000
1	3.402583000	0.147875000	0.279784000
8	1.814645000	-0.229544000	1.237212000
1	1.976502000	-1.209256000	1.288358000
1	1.126503000	-0.162243000	0.532398000
8	-4.242419000	2.734097000	-0.366189000
1	-3.669707000	2.942368000	-1.125113000
1	-3.646694000	2.891633000	0.394762000
8	2.433090000	-2.629452000	-2.485035000
1	2.313636000	-1.676898000	-2.672805000
1	1.611240000	-2.846764000	-2.006036000
8	-2.341318000	0.043262000	-2.427903000

1	-2.264489000	0.998261000	-2.605331000
1	-3.003196000	-0.009474000	-1.702155000
8	2.009948000	2.649186000	1.509241000
1	2.117289000	1.685045000	1.599288000
1	2.755582000	2.906222000	0.906484000
8	0.154421000	-3.007322000	3.369643000
1	-0.644339000	-3.113047000	2.813237000
1	0.087013000	-2.091758000	3.693396000
8	-1.867925000	-2.971382000	1.314563000
1	-1.201745000	-3.039719000	0.596153000
1	-1.952386000	-1.997488000	1.410646000
8	1.857185000	3.063202000	-2.449884000
1	1.945413000	2.108885000	-2.660282000
1	1.145826000	3.043482000	-1.783684000
8	-0.071953000	2.574444000	-0.299010000
1	-0.069062000	1.563668000	-0.422610000
1	0.662031000	2.728589000	0.344010000

**OH(H<sub>2</sub>O)<sub>26</sub>  
26w-I**

1	-0.152279000	1.048507000	-0.009570000
8	0.031708000	0.079182000	-0.019332000
8	-3.923544000	-0.908710000	0.385305000
1	-3.335331000	-0.695502000	-0.373338000
1	-3.319787000	-0.805214000	1.144091000
8	-1.282835000	-3.255698000	1.805660000
1	-2.026641000	-3.587817000	1.249130000
1	-1.515055000	-2.311483000	1.958770000
8	0.539340000	-2.611015000	-0.079671000
1	0.375147000	-1.639567000	-0.070121000
1	-0.085896000	-2.950561000	0.616040000
8	-2.025872000	-0.478186000	-1.656546000
1	-1.884458000	-1.425142000	-1.900204000
1	-1.257032000	-0.274730000	-1.044636000
8	2.072272000	0.281082000	1.707817000
1	1.312932000	0.178630000	1.058730000
1	2.838147000	0.517386000	1.123841000
8	3.951268000	0.908801000	-0.169080000
1	3.304327000	0.788745000	-0.896517000
1	4.011743000	1.893945000	-0.086236000
8	3.586647000	3.614549000	0.022205000
1	2.946657000	3.647583000	0.758588000
1	3.015649000	3.668320000	-0.772443000
8	1.432634000	3.101141000	1.957946000
1	1.702476000	2.161165000	1.091743000
1	0.774393000	3.123203000	1.228058000
8	-0.611575000	2.715636000	3.952253000
1	0.149104000	2.976057000	3.392752000
1	-0.369663000	1.823600000	4.254326000
8	-3.497763000	2.016411000	-2.163344000
1	-4.014582000	2.106090000	-1.332474000
1	-3.138659000	1.114369000	-2.102635000
8	-4.824388000	1.925534000	0.313669000
1	-4.180355000	2.229805000	0.979995000
1	-4.786726000	0.956036000	0.408351000
8	0.353075000	-0.149293000	3.949729000
1	0.486595000	-1.111114000	4.117862000
1	1.095104000	0.070966000	3.354628000
8	1.966424000	3.235004000	-2.282446000
1	1.944256000	2.263332000	-2.326404000
1	1.034997000	3.494543000	-2.371750000
8	-0.545930000	2.802275000	0.050051000
1	-0.753060000	2.986479000	-0.892846000
1	-1.389903000	2.741468000	0.548415000
8	-1.338460000	-3.100221000	-2.175435000
1	-0.828754000	-2.983347000	-3.010437000
1	-0.636236000	-3.084609000	-1.493545000
8	0.751604000	-2.915443000	3.896928000
1	0.031388000	-3.282688000	3.354218000
1	1.521042000	-2.940776000	3.294856000
8	0.371446000	-2.349319000	-4.240012000
1	1.245422000	-2.386313000	-3.813698000
1	0.179354000	-1.393756000	-4.307750000
8	2.512012000	-2.353124000	-2.166242000
1	1.887894000	-2.696470000	-1.501033000
1	3.355594000	-2.279119000	-1.657457000
8	-1.577502000	-0.479858000	2.007210000
1	-0.992139000	-0.329667000	2.789485000

1	-0.961924000	-0.285818000	1.232329000
8	-2.492755000	2.235047000	1.945597000
1	-2.312941000	1.273056000	1.969641000
1	-1.970689000	2.548987000	2.719415000
8	-1.029631000	3.114184000	-2.679771000
1	-1.989068000	2.930196000	-2.542697000
1	-0.759732000	2.356445000	-3.235025000
8	2.722712000	-2.465661000	1.783237000
1	2.569830000	-1.501044000	1.892958000
1	2.056612000	-2.680331000	1.099045000
8	-3.290746000	-3.725287000	-0.045013000
1	-3.708846000	-2.845603000	0.042195000
1	-2.840103000	-3.686116000	-0.906977000
8	1.828233000	0.316962000	-1.958235000
1	1.161407000	0.205745000	-1.211582000
1	2.115699000	-0.608691000	-2.145425000
8	4.601948000	-1.899417000	-0.403878000
1	4.176745000	-2.184374000	0.428024000
1	4.663498000	-0.931257000	-0.302671000
8	-0.310266000	0.486567000	-3.777217000
1	0.494213000	0.487861000	-3.213974000
1	-1.000812000	0.179430000	-3.154234000

**26w-II**

1	0.382507000	0.997963000	-0.237284000
8	0.032092000	0.103463000	-0.022069000
8	3.452155000	-0.657462000	1.841039000
1	2.586159000	-0.278565000	2.114723000
1	3.301312000	-0.874294000	0.902730000
8	1.671732000	-3.610698000	0.114293000
1	2.023955000	-3.683778000	1.032185000
1	2.046653000	-2.758770000	-0.204953000
8	-0.722312000	-2.463379000	0.588922000
1	-0.458211000	-1.540693000	0.365298000
1	0.109798000	-2.983142000	0.421959000
8	0.875502000	0.239570000	2.501705000
1	0.560181000	-0.591210000	2.935136000
1	0.523967000	0.162941000	1.560764000
8	-0.947910000	-0.350815000	-2.454741000
1	-0.593776000	-0.209490000	-1.523664000
1	-1.865902000	0.023977000	-2.404014000
8	-3.389807000	0.750177000	-1.967601000
1	-3.185223000	0.865947000	-1.015803000
1	-3.266748000	1.663954000	-2.332638000
8	-2.618123000	3.268863000	-2.689269000
1	-1.707602000	3.115667000	-3.002497000
1	-2.491989000	3.575984000	-1.764701000
8	0.131304000	2.256392000	-3.146523000
1	-0.238261000	1.364205000	-2.991412000
1	0.425739000	2.532654000	-2.252999000
8	2.707230000	1.209367000	-3.950760000
1	1.842179000	1.653961000	-3.835217000
1	2.468673000	0.268387000	-4.014211000
8	1.852818000	2.930731000	2.112808000
1	2.809715000	2.781851000	1.932301000
1	1.555485000	2.066504000	2.449976000
8	4.406106000	2.088657000	1.362729000
1	4.387658000	2.042038000	0.389391000
1	4.318786000	1.150774000	1.619336000
8	1.495619000	-1.463062000	-3.390321000
1	1.350196000	-2.433317000	-3.297395000
1	0.596082000	-1.092594000	-3.301496000
8	-2.423877000	3.619476000	0.074053000
1	-2.580756000	2.710110000	0.375637000
1	-1.782719000	3.965875000	0.728527000
8	1.268614000	2.569084000	-0.618756000
1	1.347931000	2.888969000	0.304052000
1	2.175405000	2.256090000	-0.840471000
8	-0.166496000	-2.152117000	3.371232000
1	-1.015557000	-1.865581000	3.784360000
1	-0.435806000	-2.389274000	2.460423000
8	0.842290000	-4.078859000	-2.674912000
1	1.190959000	-4.215709000	-1.776543000
1	-0.112136000	-3.925683000	-2.527665000
8	-2.609055000	-1.051898000	4.066488000
1	-3.155533000	-1.269290000	3.290865000
1	-2.396277000	-0.104326000	3.948300000
8	-3.414112000	-1.757096000	1.289009000
1	-2.589467000	-2.247384000	1.120237000

1	-3.911473000	-1.855865000	0.441374000
8	2.298921000	-1.049550000	-0.794648000
1	2.128676000	-1.198453000	-1.758230000
1	1.439319000	-0.624099000	-0.485854000
8	3.671133000	1.389347000	-1.353103000
1	3.339681000	0.499552000	-1.114902000
1	3.511847000	1.415810000	-2.325617000
8	-0.742396000	4.224860000	2.280911000
1	0.212589000	4.041920000	2.242402000
1	-1.081598000	3.488609000	2.822771000
8	-1.782032000	-3.007223000	-2.021840000
1	-1.493199000	-2.117770000	-2.325585000
1	-1.535224000	-2.961384000	-1.075941000
8	2.491520000	-3.273592000	2.748656000
1	2.964079000	-2.429403000	2.612175000
1	1.685402000	-3.013704000	3.229261000
8	-2.446110000	0.768702000	0.716271000
1	-1.514381000	0.520285000	0.432128000
1	-2.852544000	-0.091411000	0.977316000
8	-4.394178000	-1.886416000	-1.298379000
1	-3.661886000	-2.389061000	-1.704261000
1	-4.292698000	-0.995972000	-1.683527000
8	-1.590679000	1.567582000	3.282269000
1	-1.977182000	1.405487000	2.393580000
1	-0.688378000	1.207850000	3.169969000

**26w-III**

1	0.010736000	1.015798000	-0.333547000
8	-0.032953000	0.070743000	-0.055812000
8	2.851503000	0.461848000	2.778745000
1	1.881153000	0.607967000	2.741174000
1	3.053882000	0.185975000	1.866134000
8	2.387396000	-2.967408000	1.051368000
1	2.483935000	-2.883216000	2.029169000
1	2.603380000	-2.062631000	0.725062000
8	-0.246997000	-2.550715000	0.699719000
1	-0.177388000	-1.610486000	0.413518000
1	0.704119000	-2.814279000	0.838643000
8	0.032158000	0.601198000	2.548873000
1	-0.152432000	-0.258718000	2.999138000
1	0.003038000	0.368297000	1.569228000
8	-0.043270000	-0.803251000	-2.576890000
1	-0.030635000	-0.511845000	-1.614606000
1	-0.991080000	-0.668733000	-2.825531000
8	-2.731346000	-0.299102000	-2.868087000
1	-2.845577000	-0.086918000	-1.917664000
1	-2.704670000	0.591544000	-3.293370000
8	-2.297417000	2.304802000	-3.679774000
1	-1.319960000	2.330839000	-3.697462000
1	-2.532943000	2.779001000	-2.862445000
8	0.595804000	1.938068000	-3.327141000
1	0.440138000	0.986527000	-3.164239000
1	0.529545000	2.327389000	-2.427759000
8	3.482481000	1.672562000	-3.205404000
1	2.540881000	1.849721000	-3.390206000
1	3.521843000	0.702138000	-3.171956000
8	0.370307000	3.397469000	1.864340000
1	1.349345000	3.533321000	1.948763000
1	0.237177000	2.529437000	2.285694000
8	3.087814000	3.385913000	1.997209000
1	3.374482000	3.165772000	1.083500000
1	3.237230000	2.545428000	2.465229000
8	2.792330000	-1.226302000	-2.631534000
1	2.858524000	-2.188346000	-2.430090000
1	1.853049000	-1.116097000	-2.870250000
8	-2.872775000	2.921903000	-0.863530000
1	-2.873095000	3.423986000	-0.014013000
1	-3.066516000	2.006743000	-0.591339000
8	-0.087337000	2.769925000	-0.791418000
1	-1.059474000	2.900356000	-0.843537000
1	0.164886000	3.105689000	0.099358000
8	-0.565172000	-1.928006000	3.469369000
1	-1.538029000	-1.868829000	3.614843000
1	-0.506101000	-2.289536000	2.561483000
8	2.583309000	-3.867990000	-1.736205000
1	2.660934000	-3.819888000	-0.766565000
1	1.625349000	-3.990376000	-1.882161000
8	-3.312757000	-1.511590000	3.365865000
1	-3.546568000	-1.902428000	2.505846000

1	-3.306878000	-0.549319000	3.193457000
8	-3.124087000	-2.514205000	0.568480000
1	-2.190744000	-2.762648000	0.701559000
1	-3.301844000	-2.808870000	-0.357330000
8	2.595831000	-0.407659000	-0.000107000
1	2.784735000	-0.649728000	-0.939559000
1	1.613714000	-0.204618000	-0.015176000
8	3.790246000	2.200420000	-0.414554000
1	3.411888000	1.323310000	-0.222481000
1	3.757992000	2.226953000	-1.392175000
8	-2.499240000	3.992484000	1.666759000
1	-1.535058000	4.077802000	1.784067000
1	-2.703221000	3.171439000	2.156387000
8	-0.324423000	-3.547470000	-1.987291000
1	-0.163726000	-2.641051000	-2.331801000
1	-0.377447000	-3.371429000	-1.025752000
8	2.353529000	-2.251973000	3.732427000
1	2.616901000	-1.319295000	3.599051000
1	1.404512000	-2.198582000	3.942129000
8	-2.692786000	0.140086000	-0.054092000
1	-1.686056000	0.090084000	-0.047789000
1	-2.964248000	-0.776361000	0.194440000
8	-3.206681000	-3.087383000	-2.141036000
1	-2.288699000	-3.402862000	-2.256014000
1	-3.212475000	-2.232283000	-2.608296000
8	-2.760224000	1.241881000	2.548141000
1	-2.851203000	0.937492000	1.618856000
1	-1.799246000	1.116368000	2.696848000

**26w-IV**

1	0.154679000	1.009388000	-0.377888000
8	-0.042883000	0.091782000	-0.075806000
8	2.739067000	0.048024000	2.830834000
1	1.820327000	0.375885000	2.866394000
1	2.839008000	-0.223581000	1.899181000
8	1.923253000	-3.287821000	1.050279000
1	2.056099000	-3.244452000	2.027201000
1	2.258179000	-2.414161000	0.740626000
8	-0.624331000	-2.479494000	0.701818000
1	-0.420978000	-1.559196000	0.415666000
1	0.277997000	-2.876805000	0.845605000
8	-0.035253000	0.762471000	2.491250000
1	-0.945013000	1.120608000	2.639574000
1	-0.053701000	0.482164000	1.523027000
8	-0.177870000	-0.800456000	-2.596488000
1	-0.125094000	-0.505824000	-1.638078000
1	-1.096298000	-0.531308000	-2.846671000
8	-2.763325000	0.092565000	-2.888286000
1	-2.847123000	0.317596000	-1.937116000
1	-2.599111000	0.970357000	-3.308456000
8	-1.925586000	2.604997000	-3.683511000
1	-0.956262000	2.480816000	-3.723329000
1	-2.067116000	3.117446000	-2.868151000
8	0.885710000	1.796347000	-3.388749000
1	0.585790000	0.880229000	-3.225362000
1	0.869376000	2.193692000	-2.489539000
8	3.706665000	1.121860000	-3.168387000
1	2.808809000	1.438262000	-3.388952000
1	3.593973000	0.157669000	-3.122158000
8	0.976266000	3.337231000	1.737331000
1	1.957867000	3.337140000	1.869074000
1	0.709781000	2.467928000	2.098987000
8	3.653557000	2.885512000	2.017745000
1	3.907500000	2.592248000	1.114379000
1	3.615689000	2.044772000	2.505256000
8	2.574612000	-1.621434000	-2.575954000
1	2.501777000	-2.585538000	-2.383989000
1	1.666799000	-1.380637000	-2.838587000
8	-2.377526000	3.316610000	-0.839810000
1	-2.286094000	3.770449000	0.031004000
1	-2.719460000	2.435149000	-0.604166000
8	0.351992000	2.751641000	-0.876240000
1	-0.590201000	3.029788000	-0.894701000
1	0.692819000	3.073425000	-0.008848000
8	-0.771311000	-1.786595000	3.488457000
1	-0.462905000	-0.876933000	3.282280000
1	-0.808830000	-2.175987000	2.591478000
8	1.992116000	-4.211195000	-1.719683000
1	2.071236000	-4.169412000	-0.749371000

1	1.027100000	-4.196091000	-1.869821000
8	-3.545449000	-0.928464000	3.385745000
1	-3.802337000	-1.354005000	2.549312000
1	-2.675286000	-1.329771000	3.582739000
8	-3.454939000	-2.016951000	0.579420000
1	-2.563991000	-2.391795000	0.709294000
1	-3.676011000	-2.293204000	-0.342321000
8	2.472382000	-0.760256000	0.042516000
1	2.641713000	-1.035870000	-0.892101000
1	1.528707000	-0.418500000	0.001739000
8	4.135422000	1.575532000	-0.379416000
1	3.597994000	0.786707000	-0.183929000
1	4.085809000	1.620705000	-1.355735000
8	-1.791098000	4.224306000	1.720037000
1	-0.823866000	4.148965000	1.826527000
1	-2.145602000	3.503591000	-2.708800000
8	-0.840089000	-3.474370000	-1.982130000
1	-0.551731000	-2.602443000	-2.332249000
1	-0.869474000	-3.286073000	-1.022012000
8	2.037452000	-2.654353000	3.745250000
1	2.411728000	-1.759555000	3.623639000
1	1.089291000	-2.471396000	3.888824000
8	-2.664842000	0.544083000	-0.084062000
1	-1.676703000	0.349275000	-0.073574000
1	-3.064433000	-0.318525000	0.184638000
8	-3.623505000	-2.599241000	-2.129290000
1	-3.512668000	-1.758442000	-2.608824000
1	-2.760104000	-3.042930000	-2.245103000
8	-2.661934000	1.584540000	2.552089000
1	-3.087978000	0.816574000	2.997752000
1	-2.770097000	1.346654000	1.606274000

**26w-V**

1	-1.054887000	0.199830000	-0.073940000
8	-0.090308000	0.030144000	-0.021678000
8	-0.599512000	-3.582440000	-1.477044000
1	-0.427450000	-2.700689000	-1.879658000
1	-0.564666000	-3.391774000	-0.522182000
8	2.305019000	-3.103365000	0.968818000
1	2.422238000	-3.583187000	0.116027000
1	1.330408000	-2.994805000	1.036931000
8	2.616391000	-0.560175000	0.116824000
1	1.662602000	-0.330240000	0.065637000
1	2.609126000	-1.494674000	0.456213000
8	0.044736000	-1.033358000	-2.461084000
1	1.003348000	-1.192698000	-2.641813000
1	0.032971000	-0.610143000	-1.549561000
8	0.252889000	1.160037000	2.361158000
1	0.156145000	0.727072000	1.457914000
1	0.353083000	2.122352000	2.131465000
8	0.502591000	3.688295000	1.383954000
1	0.547663000	3.388554000	0.448414000
1	-0.426727000	4.014896000	1.474113000
8	-2.193907000	4.168716000	1.544051000
1	-2.487669000	3.412284000	2.079943000
1	-2.549476000	3.937756000	0.658126000
8	-2.595244000	1.318364000	2.462943000
1	-1.619042000	1.279549000	2.530635000
1	-2.759524000	1.078401000	1.532395000
8	-3.177600000	-1.269427000	3.606044000
1	-3.102188000	-0.329556000	3.346764000
1	-2.273084000	-1.486114000	3.890304000
8	-2.764005000	-0.662448000	-2.804140000
1	-3.140759000	-1.544153000	-2.577803000
1	-1.810953000	-0.845388000	-2.902632000
8	-3.483008000	-3.150923000	-1.768444000
1	-3.679744000	-2.974276000	-0.831305000
1	-2.581652000	-3.523747000	-1.732608000
8	-0.196117000	-1.364156000	3.710242000
1	0.722934000	-1.681741000	3.875774000
1	-0.067586000	-0.422182000	3.491479000
8	-3.328286000	3.070481000	-0.780678000
1	-3.018566000	2.947401000	-1.701249000
1	-3.457002000	2.157128000	-0.480116000
8	-2.964661000	0.207987000	-0.179893000
1	-2.939289000	0.011589000	-1.145730000
1	-3.188205000	-0.661596000	0.228807000
8	2.776091000	-1.332866000	-2.627564000
1	3.020699000	-0.519207000	-3.130810000

1	2.895895000	-1.052584000	-1.697899000
8	2.488396000	-2.082451000	3.741019000
1	2.634673000	-2.601545000	2.931194000
1	2.844814000	-1.200276000	3.518802000
8	3.158330000	1.192690000	-3.698890000
1	3.442981000	1.683781000	-2.909008000
1	2.230482000	1.472678000	-3.834864000
8	3.589513000	1.985719000	-0.854530000
1	3.554042000	1.076470000	-0.509064000
1	3.647646000	2.537574000	-0.038277000
8	-0.381322000	-2.328152000	1.128363000
1	-0.379004000	-2.094028000	2.088275000
1	-0.257021000	-1.430350000	0.680977000
8	-3.221876000	-2.271168000	1.003780000
1	-2.254890000	-2.427280000	1.009581000
1	-3.393350000	-2.038674000	1.944478000
8	-2.595847000	2.231466000	-3.396010000
1	-2.879482000	1.301642000	-3.373951000
1	-1.649347000	2.169226000	-3.622470000
8	2.976689000	0.602987000	2.721969000
1	2.013921000	0.803744000	2.747906000
1	3.060768000	0.243127000	1.816667000
8	2.300675000	-4.071405000	-1.643327000
1	1.331028000	-4.087293000	-1.752209000
1	2.582676000	-3.314837000	-2.187248000
8	0.830958000	2.366013000	-1.040614000
1	0.483527000	1.512622000	-0.661796000
1	1.808598000	2.258938000	-1.025198000
8	3.385768000	3.284667000	1.592466000
1	3.377751000	2.498278000	2.169757000
1	2.474299000	3.624025000	1.658681000
8	0.262845000	1.666590000	-3.641639000
1	0.409155000	2.053725000	-2.746216000
1	0.114512000	0.725807000	-3.428429000

**26w-VI**

1	-0.441452000	-0.047070000	-1.100656000
8	0.302910000	-0.063599000	-0.452003000
8	4.665725000	-2.621658000	-0.998867000
1	4.223579000	-2.796437000	-0.142705000
1	4.830999000	-1.657784000	-0.964767000
8	2.515750000	-2.783890000	-2.606778000
1	3.375735000	-2.813167000	-2.106912000
1	2.572725000	-3.457819000	-3.294690000
8	2.208894000	0.037546000	-2.325315000
1	1.478881000	-0.014420000	-1.640111000
1	2.234259000	-0.856772000	-2.713252000
8	2.575663000	2.944604000	1.187751000
1	2.696770000	1.976330000	1.266678000
1	3.218691000	3.192911000	0.480568000
8	-1.115637000	-0.295590000	1.769010000
1	-1.173003000	-1.277020000	1.865367000
1	-0.600827000	-0.191655000	0.907759000
8	0.684255000	-2.706977000	-0.471532000
1	1.245136000	-2.867663000	-1.260098000
1	0.551958000	-1.709879000	-0.462997000
8	-0.999192000	-3.047221000	1.863932000
1	-0.512360000	-3.192462000	1.031804000
1	-0.298546000	-3.092532000	2.556393000
8	1.811975000	2.829794000	-2.689124000
1	1.282291000	2.818391000	-1.869371000
1	1.954296000	1.876249000	-2.852431000
8	4.185930000	3.212251000	-1.043395000
1	4.522051000	2.296102000	-1.052562000
1	3.489992000	3.200908000	-1.731347000
8	-1.407662000	2.613251000	2.049340000
1	-0.926537000	2.691318000	1.195615000
1	-1.468568000	1.647940000	2.162735000
8	0.987327000	2.895199000	3.649791000
1	0.123900000	2.992666000	3.200433000
1	1.626146000	3.156252000	2.962702000
8	0.245639000	2.586787000	-0.227658000
1	1.048821000	2.841920000	0.289851000
1	0.297295000	1.582527000	-0.285818000
8	4.487367000	0.273891000	-0.806758000
1	3.698878000	0.204461000	-1.399905000
1	4.073134000	0.254810000	0.074106000
8	1.152874000	-2.813993000	3.620680000
1	1.889311000	-2.890437000	2.983892000

1	1.170976000	-1.873396000	3.873127000
8	2.905378000	-2.705952000	1.279591000
1	2.911797000	-1.726878000	1.334656000
1	2.112649000	-2.851181000	0.716133000
8	2.445714000	0.092997000	1.271503000
1	1.989108000	0.088536000	2.156037000
1	1.699445000	0.035842000	0.630942000
8	0.991232000	0.120747000	3.540920000
1	1.022665000	1.081342000	3.763911000
1	0.152009000	0.024683000	3.035098000
8	-3.866015000	-2.975669000	1.162170000
1	-4.062122000	-2.046421000	1.375397000
1	-2.974267000	-3.119879000	1.523080000
8	-1.693633000	0.087795000	-2.380637000
1	-2.617144000	0.007524000	-2.025905000
1	-1.602501000	1.027445000	-2.625071000
8	-1.416995000	-2.739030000	-2.615835000
1	-0.830589000	-2.870435000	-1.851615000
1	-1.403290000	-1.771023000	-2.739814000
8	-4.136860000	-2.934465000	-1.686808000
1	-4.038158000	-3.094812000	-0.725349000
1	-3.224044000	-3.007221000	-2.031327000
8	-4.241544000	2.686808000	1.276541000
1	-3.334606000	2.905863000	1.557865000
1	-4.223521000	2.801814000	0.302744000
8	-1.360578000	2.949162000	-2.533136000
1	-0.654984000	3.184304000	-3.154368000
1	-0.910345000	2.988618000	-1.666044000
8	-4.200352000	-0.203500000	-1.415889000
1	-4.122674000	-0.183176000	-0.433173000
1	-4.331217000	-1.163388000	-1.614539000
8	-3.903803000	-0.050952000	1.323250000
1	-4.150220000	0.900846000	1.417270000
1	-2.935846000	-0.061098000	1.468146000
8	-4.193200000	2.650001000	-1.569090000
1	-4.336609000	1.696379000	-1.719042000
1	-3.369361000	2.851350000	-2.041679000

**26w-VII**

8	0.600095000	-0.085387000	0.029172000
8	-0.091014000	-0.980573000	2.518846000
8	2.117890000	2.013529000	0.773906000
8	-2.268642000	-1.622411000	-0.711856000
8	-0.075803000	0.988316000	-2.428387000
8	-2.165365000	-0.727537000	-3.355091000
8	-0.604902000	-2.948687000	-3.818545000
8	-2.342052000	-2.429831000	2.068837000
8	0.123762000	3.889428000	1.088493000
8	-1.944289000	2.904786000	-1.887589000
8	0.455939000	4.644330000	-1.544841000
8	-4.040145000	1.292213000	-2.624978000
8	-4.028520000	-0.427837000	2.991395000
8	1.700451000	-1.185976000	-3.337019000
8	-1.630089000	1.216764000	3.345063000
8	-1.671002000	1.647603000	0.698037000
8	0.377670000	3.011978000	3.873719000
8	2.208256000	0.807895000	3.269184000
8	-4.121040000	0.282860000	0.152154000
8	2.330194000	2.497038000	-2.013519000
8	4.120275000	0.567626000	-2.829527000
8	1.889146000	-2.979660000	1.858184000
8	1.882374000	-2.291302000	-0.824438000
8	-0.459232000	-4.708139000	1.556311000
8	-0.435836000	-3.565963000	-1.018338000
8	3.796777000	-0.359878000	-0.228575000
8	4.220493000	-1.280187000	2.451378000
1	1.118403000	-0.866959000	-0.293254000
1	2.332936000	1.150763000	2.357665000
1	1.495278000	0.152053000	3.180997000
1	-1.020449000	1.921901000	3.674257000
1	-1.044757000	0.434085000	3.252200000
1	-1.076840000	0.931879000	0.400030000
1	-1.711363000	1.524805000	1.687738000
1	1.480069000	2.756914000	0.880742000
1	-2.350632000	-1.300729000	-1.637499000
1	-1.399827000	-0.144056000	-3.180396000

1	-1.736869000	-1.560629000	-3.669898000
1	-0.606170000	-3.394735000	-2.949087000
1	0.258230000	-2.489748000	-3.827712000
1	0.461666000	-3.125401000	-0.935897000
1	0.383393000	-4.274514000	1.798500000
1	-1.140286000	-4.142307000	1.958215000
1	4.149029000	-0.596421000	0.653168000
1	3.166452000	-1.090756000	-0.422309000
1	3.555602000	-1.989337000	2.350497000
1	3.733005000	-0.592127000	2.937561000
1	-3.011440000	-1.851015000	2.505575000
1	-2.473030000	-2.241042000	1.120354000
1	1.131122000	-0.401779000	-3.261948000
1	1.741538000	-1.546216000	-2.409904000
1	2.560194000	-2.920407000	-1.115905000
1	0.232474000	4.329118000	0.211574000
1	-0.576347000	3.228465000	0.926539000
1	-3.404702000	0.251461000	3.304808000
1	-4.287143000	-0.111662000	2.103777000
1	-0.327820000	4.244837000	-1.959897000
1	1.202588000	4.090940000	-1.845904000
1	-2.009994000	2.727442000	-0.932475000
1	-2.750107000	2.452845000	-2.245905000
1	-0.882038000	-1.572729000	2.424231000
1	0.078014000	-0.683870000	1.591748000
1	1.284984000	-2.316250000	2.243307000
1	1.892417000	-2.745169000	0.892307000
1	4.235104000	0.237931000	-1.912026000
1	3.487215000	-0.073210000	-3.203512000
1	-3.652867000	-0.540889000	-0.093884000
1	-3.359919000	0.875828000	0.315472000
1	1.126548000	2.387734000	3.795887000
1	0.429001000	3.548213000	3.062497000
1	0.046907000	0.580670000	-1.540030000
1	-0.727910000	1.719504000	-2.283286000
1	-4.313628000	0.944597000	-1.754446000
1	-3.598434000	0.529558000	-3.045216000
1	3.072347000	1.970833000	-2.399283000
1	1.549676000	1.959866000	-2.257142000
1	1.274992000	0.600461000	0.279974000
1	2.510398000	2.152839000	-0.113713000
1	-1.600623000	-2.353470000	-0.804551000
1	-0.489506000	-4.148117000	-0.230355000

**26w-VIII**

1	2.108451000	-0.181468000	-2.707930000
8	2.068899000	-0.105631000	-1.742122000
8	4.939005000	2.774612000	1.361700000
1	5.044966000	1.829808000	1.598973000
1	3.992591000	2.935301000	1.545231000
8	5.087566000	2.728909000	-1.317420000
1	5.109674000	2.818199000	-0.325142000
1	5.751885000	3.345580000	-1.647193000
8	2.239029000	2.536807000	-1.321064000
1	2.196823000	1.557743000	-1.525091000
1	3.164654000	2.777179000	-1.516395000
8	-0.742364000	0.254379000	1.474863000
1	0.228846000	0.159858000	1.564030000
1	-0.882975000	1.236582000	1.466250000
8	1.986980000	-2.834887000	-1.286908000
1	2.940666000	-3.081660000	-1.350295000
1	2.011650000	-1.863062000	-1.472250000
8	4.755044000	-0.138353000	-1.197638000
1	5.046197000	0.763061000	-1.428479000
1	3.785563000	-0.133082000	-1.413394000
8	4.732021000	-3.073817000	-1.115252000
1	4.993305000	-2.150171000	-1.275268000
1	4.761872000	-3.148162000	-0.136783000
8	-0.607991000	2.807091000	-1.503579000
1	-0.631269000	1.829078000	-1.563038000
1	0.336338000	3.005268000	-1.647101000
8	-0.860453000	2.969413000	1.280500000
1	0.077155000	3.132394000	1.502032000
1	-0.869330000	3.048914000	0.299996000
8	-0.881273000	-2.864982000	-1.449496000
1	-0.804015000	-1.894020000	-1.553335000
1	0.039248000	-3.163902000	-1.573133000
8	-1.233851000	-2.616705000	1.320019000
1	-1.226286000	-2.809454000	0.354882000

1	-1.247750000	-1.643778000	1.351384000
8	-0.524373000	-0.034910000	-1.304510000
1	-0.624271000	0.031999000	-0.329441000
1	0.471652000	-0.061773000	-1.476371000
8	2.026966000	2.700930000	1.409251000
1	2.085123000	2.691931000	0.420848000
1	2.018794000	1.750469000	1.616567000
8	4.528240000	-3.022830000	1.705472000
1	4.733238000	-2.085398000	1.877345000
1	3.571247000	-3.084573000	1.868609000
8	4.811278000	-0.079591000	1.585659000
1	3.835693000	-0.065138000	1.647932000
1	4.920807000	-0.149834000	0.608241000
8	2.001769000	-0.224258000	1.125970000
1	1.871887000	-1.198349000	1.310380000
1	2.078289000	-0.187757000	0.150746000
8	1.599722000	-2.845690000	1.411729000
1	0.638526000	-2.942450000	1.577585000
1	1.682069000	-2.986788000	0.434885000
8	-3.592706000	2.816807000	2.384208000
1	-2.690337000	3.072211000	2.129343000
1	-4.124926000	2.995526000	1.571807000
8	-4.840062000	0.132847000	-0.016662000
1	-4.188265000	0.142200000	-0.751059000
1	-4.304134000	0.054999000	0.800505000
8	-3.183332000	0.051301000	-2.286527000
1	-2.233909000	0.018918000	-2.072260000
1	-3.401952000	-0.892546000	-2.493768000
8	-5.340639000	-2.683263000	-0.291094000
1	-4.940643000	-2.899659000	0.575643000
1	-5.404427000	-1.709380000	-0.234030000
8	-3.455684000	2.948552000	-2.302704000
1	-3.487960000	1.991926000	-2.488888000
1	-2.508881000	3.115177000	-2.163952000
8	-4.018399000	-2.826685000	2.252106000
1	-4.076360000	-1.890338000	2.510638000
1	-3.077804000	-2.923068000	2.017335000
8	-3.493781000	0.087045000	2.486464000
1	-2.530153000	-0.009647000	2.425621000
1	-3.603826000	1.069352000	2.570345000
8	-5.084713000	2.986185000	0.062666000
1	-5.230648000	2.019892000	0.023998000
1	-4.544690000	3.136038000	-0.739509000
8	-3.646166000	-2.639390000	-2.478449000
1	-2.791968000	-3.018610000	-2.213642000
1	-4.236288000	-2.786622000	-1.700830000