

Electronic Supplementary Information for article:

Infrared spectroscopy of O^{•-} and OH⁻ in water clusters: Evidence for fast interconversion between O^{•-} and OH[•]OH⁻

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Experimental methods

The IRMPD experiments are performed using a 4.7 T Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometer (Bruker/Spectrospin CMS47X) equipped with a tunable optical parametric oscillator (OPO; EKSPLA NT277). A detailed description of the FT-ICR can be found elsewhere.^{1,2} The reactant ions, (H₂O)_n^{•-}, are produced by laser vaporization of a solid zinc target and supersonic expansion of water vapor with He as a buffer gas through a nozzle into the vacuum.^{3,4} The anionic water clusters are transferred from the ion source via an electrostatic lens system through differential pumping stages into the ICR cell with a background pressure below 8×10⁻¹⁰ mbar, in which the ions are stored. N₂O is introduced through a leak valve at constant pressures at around 1 × 10⁻⁸ mbar. The reactions of anionic water clusters with N₂O produce both (H₂O)_nO^{•-} and (H₂O)_nOH⁻ product ions.^{5–7} The reaction and the purity of product ions are monitored by recording mass spectra at different reaction delays.

(H₂O)_nO^{•-} and (H₂O)_nOH⁻ clusters are irradiated at specific frequencies with tunable IR laser radiation. The laser radiation is introduced through a CaF₂ window at

the rear end of the vacuum system into the ICR cell. The diode pumped Q-switched laser, operated at 1000 Hz repetition rate with pulse duration of approximately 6-9 ns, provides a bandwidth of 8 cm^{-1} for the IR radiation. The system offers tuning from 2400 to 4000 cm^{-1} and produces pulses with energy of $\sim 90\text{-}190 \mu\text{J}$, measured at the chamber entrance. To eliminate water absorption, the relative humidity is lowered by introducing dry nitrogen along the IR laser beam pathway.

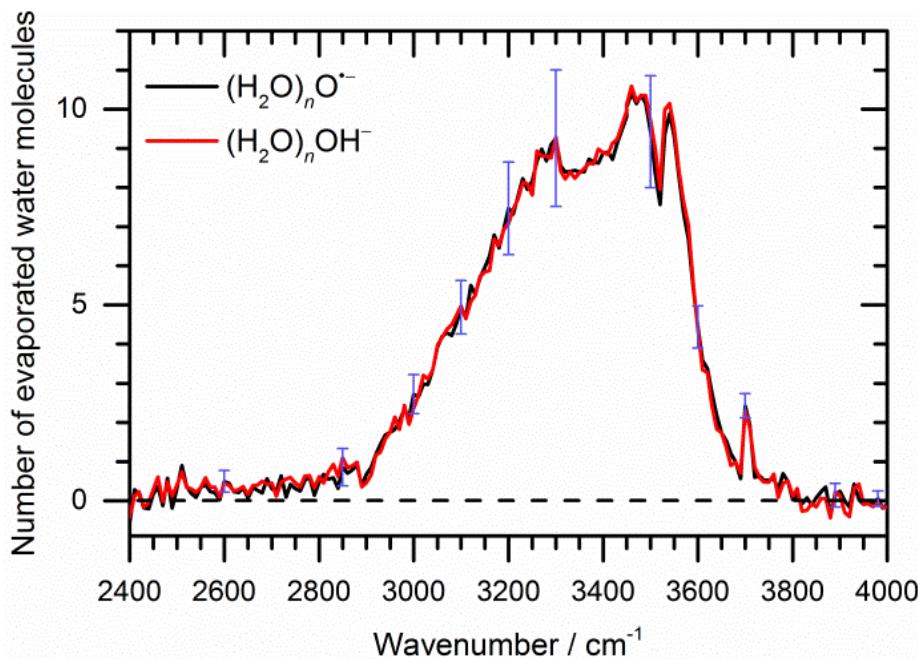


Figure S1. Raw IRMPD spectra of $(\text{H}_2\text{O})_n\text{O}^{\bullet-}$ and $(\text{H}_2\text{O})_n\text{OH}^-$ cluster ions, $\bar{n} \approx 47$, measured in the range of $2400\text{-}4000 \text{ cm}^{-1}$, with the number of evaporated water molecules per second as a function of the irradiation energy. Note that different shape of the spectrum with respect to Figure 1 is caused by the changes of laser pulse energy with wavelength. The quality of the correction can be judged by the removal of the pronounced dip around 3520 cm^{-1} .

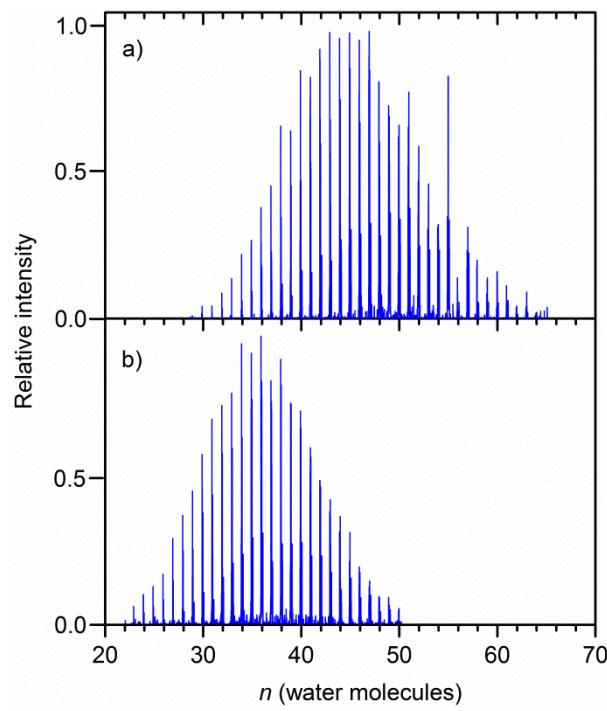


Figure S2. A typical mass spectrum as retrieved after 1 second of storage in the ICR cell, a) without irradiation and b) with irradiation at 3500 cm^{-1} .

Evaluating the relative probability of H₂O and OH[•] evaporation

The relative activation energy of OH[•] evaporation with respect to H₂O evaporation is derived based on the following observations and assumptions:

- 1) Within evaporation of 10 H₂O molecules, there is a probability $p_{\text{OH}^{\bullet}}$ of 2% to evaporate an OH[•] radical.
- 2) There are on average 46 water molecules per one OH[•] in the cluster.
- 3) We assume that the (H₂O)_{n-1}OH[•]OH⁻ isomer is exclusively present.

In the experiment, 10 water molecules are being dissociated in the 3200–3500 cm⁻¹ region, see Figure S1. We can deduce the probability $p_{\text{H}_2\text{O}}$ that in a specific evaporation event, H₂O is evaporated:

$$p_{\text{H}_2\text{O}} = (1 - 0.02)^{1/10} = 0.98^{1/10} \quad (\text{S1})$$

The probability of evaporating an OH[•] radical, $p_{\text{OH}^{\bullet}}$, is equal to the ratio of dissociation rates of OH[•] and H₂O, $k_{\text{OH}^{\bullet}}$ and $k_{\text{H}_2\text{O}}$, with the factor of 46 to correct for the number of water molecules in the cluster:

$$p_{\text{OH}^{\bullet}} = \frac{k_{\text{OH}^{\bullet}}}{46 \cdot k_{\text{H}_2\text{O}}} = 1 - 0.98^{1/10} \quad (\text{S2})$$

Finally, the ratio of the rate constants is:

$$\frac{k_{\text{OH}^{\bullet}}}{k_{\text{H}_2\text{O}}} = 46 \cdot (1 - 0.98^{1/10}) = 0.093 \quad (\text{S3})$$

Expressing $k_{\text{OH}^{\bullet}}$ and $k_{\text{H}_2\text{O}}$ via the Arrhenius equation assuming identical prefactors, the difference in activation energy is obtained:

$$\Delta E_a = -RT \ln \frac{k_{\text{OH}^{\bullet}}}{k_{\text{H}_2\text{O}}} = -RT \ln 0.093 = 2.0 \text{ kJ/mol} \quad (\text{S4})$$

With respect to assumption No. 3, we can also evaluate the energy difference when (H₂O)_{n-1}OH[•]OH⁻ and (H₂O)_nO^{•-} clusters are present in equal amount, i.e. 50%:50%. Then the ratio between the number of OH[•] and H₂O is two times smaller, i.e.

there is on average one OH[•] per 92 H₂O water molecules. Equations (S3) and (S4) then change to:

$$\frac{k_{\text{OH}^{\bullet}}}{k_{\text{H}_2\text{O}}} = 2 \cdot 46 \cdot (1 - 0.98^{1/10}) = 0.186 \quad (\text{S5})$$

$$\Delta E_a = -RT \ln \frac{k_{\text{OH}^{\bullet}}}{k_{\text{H}_2\text{O}}} = -RT \ln 0.186 = 1.4 \text{ kJ/mol} \quad (\text{S6})$$

Very small energy differences are sufficient to rationalize the preferential evaporation of H₂O, which is observed experimentally. This is due to the low internal temperature of the clusters, which is maintained by evaporative cooling.

References

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Structures optimized at the B3LYP+D2/TZVP level (coordinates in Å,
energies in Hartree)

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O 1.504981 -1.850736 -0.283075	O 2.065050 -1.426672 0.641991

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 H 0.002985 1.916676 -0.187572
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 H 2.156081 1.679340 0.083915

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 O -0.518027 2.105346 0.777660
 O 2.209144 -1.292620 0.481868
 O 0.129676 -0.342016 2.128584
 O -1.775938 -1.688385 0.601182
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 H -1.891428 0.814814 -1.103154
 H -2.523537 -0.139166 -0.085687
 H -1.454400 1.838413 0.717064
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 H 1.606757 -1.611082 -0.216686
 H 2.457054 -0.394661 0.178282
 H 1.558110 1.215163 -0.961711
 H 2.020967 1.857310 0.358794
 H -0.002487 0.542935 1.734672
 H 0.915897 -0.712801 1.674366
 H -1.179968 -1.284919 1.271178
 H -1.174666 -1.873729 -0.143213
 H 0.114526 -0.670333 -1.618026
 O 0.191354 -1.684839 -1.457696
 H 0.175644 -2.104486 -2.321779

 22
 0.7h2o, E= -610.427784
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 O -1.095104 1.868668 -1.012004
 O -2.997375 0.131235 0.330758
 O 1.931109 -1.837559 0.311320
 O 0.527270 1.752190 1.243766
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 H 2.919874 0.063207 0.152167
 H 1.534132 -1.420170 -0.484266
 H 1.303903 -1.609002 1.019055
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 H -0.515317 1.177694 -1.413503
 H -1.861498 1.382490 -0.657552

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 H -2.513081 0.110681 1.167810

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 H 3.203113 -0.047640 0.975968
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 H 2.170710 1.155008 -0.645981
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 O 3.290510 -0.168958 0.240355
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 O 2.002255 1.497011 1.069655
 O -0.505169 0.665633 -1.740627
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 O -1.577769 -1.657997 -0.237381
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 H 2.085255 0.778771 1.707376
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 H -2.899039 0.978693 -1.004528
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 H 0.743840 -1.222471 1.313718
 H -1.152527 -1.579038 0.639436
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o.7h2o, E= -610.425498
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 H -0.620660 1.667862 1.245951
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 H 0.409231 -0.054018 1.969526

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 O 2.636891 -1.547804 -0.426506
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 H 3.357227 -1.000605 -0.755823
 O 0.538593 -0.353655 -1.526089
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22

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 O -2.697450 0.411793 -1.482728
 H -2.981054 1.201458 -1.009142
 H 1.693022 0.448282 -1.476158
 O 2.681407 0.402616 -1.485741
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H -2.879374 -0.224232 1.396198

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o 8h2o, E= -686.885926
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O 0.411539 -1.238434 -0.613670
O 2.945261 -0.868793 -1.400767

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o 8h2o, E= -686.885632
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O -1.913441 -0.750990 1.881054
H -0.959698 -0.915340 1.951838
H 3.350884 -1.767272 -0.368584
O 3.578953 -1.026949 0.203338
H 3.260740 -0.241145 -0.298591
H 0.637555 -0.958867 0.305055
O 0.893070 -0.952807 1.267379
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o 8h2o, E= -686.884893
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O 2.424121 0.349229 1.276957
O 1.416777 2.095139 -0.588124
O -1.030236 2.211052 0.828854
H -0.082171 -1.202659 -0.967922
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 O 1.765386 -1.679865 0.765777
 O -0.097915 -0.240487 -2.181545
 O 2.570515 -0.116936 -1.364289
 O 1.931248 2.211628 0.080982
 O -3.510360 1.100105 -0.665455
 O -1.865219 -0.507377 1.334643
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 H -2.556181 1.296182 -0.714611
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 O -0.826097 -2.307070 -0.322920
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 O 2.988009 -1.501903 0.227645
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 O 1.198075 2.339764 0.846262
 O -0.864877 0.554302 1.895079
 O -2.057008 1.827481 -0.286117
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 H -2.551980 -1.171887 -0.843678
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O	-1.974874	-0.553295	-1.801042	H	3.874184	-0.980135	-1.192435
O	-3.235956	0.636389	0.524831	H	2.479474	-1.319863	-0.597106
O	1.931069	2.638286	-0.608723	H	3.337220	0.370388	0.568115
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H 1.052745 1.526607 2.610900
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 H 1.533110 0.504134 1.663298
 H 1.696804 1.839231 2.519941
 H 2.375126 -0.825642 0.403396
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 H 0.523178 2.058660 -1.223342
 H 1.459429 2.030720 -0.006836
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 H -1.524708 1.855296 0.449399
 H 0.058219 -2.476874 -0.083975
 H -0.864902 -2.093865 1.110569
 H -1.569191 0.875433 -1.524604
 H -1.816077 2.387183 -1.982639
 H -3.135517 -1.033061 1.811216
 H -2.079309 0.022963 1.331159
 H 1.742523 -1.073969 -1.592873
 H 2.219752 0.402075 -1.363018
 H -2.315681 -0.864835 -0.786880
 H -1.070313 -1.158467 -1.738995

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o 9h2o, E= -763.344175
 O 2.431505 -0.367582 1.861956
 O 3.358000 0.680179 -0.724561
 O 1.081958 1.979435 -0.530060
 O -0.145812 0.535326 1.376302
 O -2.973269 -0.505344 1.546568
 O -2.824681 -1.695240 -1.057435
 O -0.193851 -1.433060 -0.387511
 O 2.500422 -2.003083 -0.389991
 O -2.284319 1.958214 0.353341

H 1.500792 -0.042286 1.766998
 H 2.941266 0.195101 1.259763
 H 4.022223 1.261210 -1.104021
 H 2.497164 1.194698 -0.730222
 H 0.693412 1.623524 0.311873
 H 0.410634 1.751787 -1.202227
 H -2.019479 -0.335756 1.655948
 H -3.040152 -1.006581 0.711489
 H -1.880915 -1.877062 -0.867631
 H -2.772904 -0.913272 -1.623712
 H 0.731198 -1.745290 -0.514655
 H -0.182019 -0.910706 0.453257
 H -1.471894 1.682906 0.839460
 H -2.921397 1.311927 0.705827
 H 2.893274 -1.223849 -0.820159
 H 2.518724 -1.718836 0.548736
 H -0.754670 -0.000338 -1.463624
 O -1.138271 0.790828 -1.891548
 H -1.658701 1.235439 -1.183594

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o 0.9h2o, E= -763.343567
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 O 1.878352 2.130457 0.042022
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 O 0.065576 -0.501169 -1.772742
 O -2.243686 -2.026330 -0.797996
 O -3.843221 -0.080177 0.476217
 O -1.825655 1.538306 1.196326
 O 0.676254 0.317143 1.889865
 O 2.904211 -1.600197 1.071200
 H -0.481326 1.113887 -1.635474
 H 0.205840 2.298459 -0.919807
 H 2.583283 2.748838 0.250197
 H 2.281907 1.385829 -0.507682
 H 1.717091 -0.221021 -1.596272
 H 2.871722 -0.614992 -0.590309
 H -1.636018 -1.459203 -1.312417
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 H -1.462835 1.762667 0.305085
 H 2.066095 -2.056099 0.852810
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 H 1.083711 0.971227 1.290810
 H 0.464642 -0.469209 1.340147
 O 0.315283 -1.986645 0.325663
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 H -0.597606 -2.326779 0.336071

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o 0.9h2o, E= -763.343182
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 O -3.112223 -0.218437 1.124588
 O -2.750072 -2.372748 -0.757376
 O -0.444084 -0.969328 -0.923537
 O 2.067323 -2.076297 -0.759993
 O -0.467759 1.726909 -1.888020

H 1.119211 -0.538296 1.716696
 H 2.648596 -0.532995 1.487833
 H 4.282388 0.808264 -0.407065
 H 2.735075 0.996763 -0.190268
 H 0.920620 1.584489 0.727285
 H 0.898486 2.032843 -0.749878
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 H -1.894697 -1.919444 -0.959199
 H -2.499306 -3.107378 -0.188672
 H 0.433576 -1.408368 -1.019920
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 H -1.170347 2.042679 -1.279039
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 H 2.671791 -1.329000 -0.915506
 H 1.984487 -2.036378 0.217398
 H -1.407804 1.885814 0.824510
 O -2.110466 2.314507 0.287529
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o 0.9h2o, E= -763.341708
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 O 0.670550 -1.792748 0.806939
 O 3.025539 1.262420 0.660869
 O -1.818274 -1.037926 -1.951258
 H -0.321028 -0.544249 1.989744
 H -1.281006 0.696301 1.971868
 H 2.853327 1.282210 1.606816
 H 2.158831 1.566512 0.232139
 H 0.638268 -1.291154 -0.042545
 H -0.113858 -2.359045 0.776484
 H -1.964063 2.116635 0.468889
 H -0.506537 2.327336 0.762835
 H -0.845498 -0.979377 -1.995920
 H -2.005656 -1.429960 -1.078985
 H -1.010431 1.867703 -1.337554
 H -2.065136 0.805877 -1.700819
 H 1.841547 -0.730497 -1.550386
 H 0.877077 0.501414 -1.289664
 H -3.065826 -2.430626 0.955469
 H -1.994144 -1.332732 1.312960
 O 3.349488 -1.265564 -0.389373
 H 3.348891 -0.366637 0.014803
 H 2.732168 -1.764166 0.164848

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 O 0.592242 -0.027779 -1.717581
 O 0.540600 -2.437815 -0.189292
 O -2.389582 2.094655 -0.004535
 O -2.300364 0.165852 -2.002725
 O -2.226229 -1.710836 0.047083
 O -1.714469 0.032613 2.190072
 O 3.111825 -0.813607 -0.508294

O 2.974261 2.187397 -0.078464
 H 2.389236 -0.499759 -1.083932
 H 2.736528 -0.796695 0.384848
 H 2.024988 2.025157 0.057603
 H 3.332578 1.305698 -0.251929
 H -1.084724 0.635711 1.755121
 H -1.938434 -0.622314 1.493276
 H -1.413044 2.037681 0.152235
 H -2.749508 1.616199 0.754674
 H 0.520783 0.673512 -1.020276
 H 0.342608 -0.854545 -1.264737
 H 0.900024 0.217383 1.305152
 H 0.546030 -0.784127 2.435007
 H 1.393162 -2.688677 -0.563456
 H 0.771253 -1.865478 0.586848
 H -1.413742 -2.206845 -0.132987
 H -2.343071 -1.121122 -0.732291
 H -2.441159 0.929780 -1.400059
 H -1.349690 0.196164 -2.205195

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o 0.9h2o, E= -763.341019
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 O -2.845050 -0.135642 1.573590
 O -2.342279 2.044731 -0.077574
 O -1.099815 0.256483 -1.816857
 O 0.675200 2.124830 -0.490196
 O 3.080799 0.676945 -1.272581
 O -3.026813 -1.898140 -0.769228
 O 1.890101 -1.908112 -0.801129
 O 3.416516 -0.645198 1.241165
 H -2.156480 -1.898406 -0.322382
 H -2.855823 -1.355930 -1.550044
 H -1.994338 -0.601177 1.376213
 H -3.443313 -0.580034 0.953708
 H 0.328866 -0.221881 1.347693
 H 0.436632 0.759159 2.597360
 H 0.993772 -1.728085 -0.457489
 H 2.165792 -1.081067 -1.239759
 H 3.408273 0.422316 -0.388716
 H 2.401012 1.351711 -1.101809
 H 0.214431 1.515805 -1.098059
 H 0.777116 1.627800 0.347634
 H -0.812308 -0.427731 -1.180601
 H -1.722206 0.823299 -1.312501
 H -2.520070 1.403933 0.645940
 H -1.452377 2.398980 0.067660
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 H 2.641864 -0.204827 1.634959

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o 0.9h2o, E= -763.340353
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 O 0.825384 -1.545390 2.166231
 O 0.228768 -0.248277 -2.247234
 O -0.520565 0.797078 2.287045
 O 0.674410 2.444627 0.651408
 O -1.288352 1.759144 -1.215495
 O -2.763294 0.538331 0.609091
 O 2.423072 1.176625 -1.212482

O -2.557862 -2.045563 -0.814499
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 H -2.271996 1.008439 -0.126776
 H -1.379062 0.626329 1.853164
 H -0.046105 -0.075673 2.312689
 H -2.762488 -1.256499 -0.291301
 H -1.592264 -2.157854 -0.678637
 H -0.789335 1.028241 -1.658666
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 H 1.716974 -1.309655 1.844522
 H 0.455914 -1.960505 1.351181
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 H 1.892442 1.657031 -0.551596
 H 2.045305 -1.628501 -0.138267
 H 2.907348 -0.364382 -0.211121
 H -0.158288 -0.615947 -3.046848
 H 0.233167 -1.031684 -1.538268
 H 0.928532 3.231636 1.140032
 H 0.267232 1.805202 1.319790

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o 0.9h2o, E= -763.339953
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 O 3.092193 -1.525077 -0.796792
 O 0.449011 -1.994906 -0.415039
 O -0.330306 -1.260566 2.097033
 O -0.209726 0.309291 -2.051774
 O -2.801287 0.073782 -1.086755
 O -2.103369 2.172191 0.659683
 O -2.233171 -2.336665 0.085367
 H 2.106121 0.986626 1.028485
 H 3.014574 0.190786 0.040038
 H -0.129001 -0.251500 1.986964
 H 0.121977 -1.545362 2.895576
 H -2.559828 -1.503698 -0.336125
 H -1.881652 -2.043401 0.940833
 H -1.309899 1.778076 1.110611
 H -1.712835 2.762881 0.005174
 H -2.737173 0.778064 -0.410297
 H -1.952875 0.170339 -1.574073
 H 0.145477 1.133258 -1.655643
 H 0.151245 -0.414321 -1.509828
 H 3.465125 -2.150053 -0.167914
 H 2.140716 -1.764606 -0.841784
 H 0.356658 -1.727864 0.527532
 H -0.451941 -2.341717 -0.588212
 H 0.549669 2.226962 0.213854
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 H 1.756065 2.321510 -0.673035

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o 0.10h2o, E= -839.808945
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 O -0.060639 -0.859297 -1.827858
 O 2.587497 -0.095623 -1.715382
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 O 0.576023 -2.275215 0.377646
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 O -3.260714 -0.425957 1.050770

O 3.077201 -1.226987 0.783265
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 H 2.484741 0.833647 -1.455879
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 H -1.623292 -2.764281 -0.200857
 H -1.502763 -1.698433 -1.287765
 H -0.480639 0.564352 -1.351320
 H 1.516278 -2.078750 0.606326
 H 0.484596 -1.972707 -0.555398
 H 3.064258 -0.868332 -0.132269
 H 2.812084 -0.463100 1.334143
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 H 1.824067 3.341305 -0.753162

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o.10h2o, E= -839.808218
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 O -1.402516 0.542530 1.694463
 O -1.726522 1.540768 -1.052123
 O 1.121618 1.734282 2.018324
 O -1.654369 -1.054796 -1.309114
 O 2.833973 -0.093152 0.993831
 O 1.668656 -2.416299 0.664673
 O 0.883736 -1.495390 -1.896085
 O 2.300464 0.671517 -1.656514
 O -1.116166 -2.116890 1.067602
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 H -3.467191 0.109194 0.911292
 H 2.823777 0.779661 -2.454955
 H 1.717644 -0.144493 -1.800889
 H 2.854799 0.244237 0.078092
 H 2.250501 0.550934 1.476268
 H 1.302311 2.105394 -1.016288
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 H -0.105232 -1.348465 -1.758113
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 H 0.250482 1.298871 2.123901
 H 1.011471 2.246325 1.185517
 H -1.418879 -1.979504 0.134722
 H -0.161546 -2.301347 0.999559
 H -1.406064 0.910619 0.792134
 H -1.273992 -0.428683 1.569785
 H -3.278290 -0.530255 -0.460106
 H -1.651186 0.582844 -1.353950
 H 2.216453 -3.106487 1.046962
 H 2.123151 -1.538623 0.860239
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o.10h2o, E= -839.807687
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O 2.463745 1.767492 0.667335
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 O 1.732992 -0.632697 2.060255
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 H 0.704483 -2.247045 -0.438133
 H 2.793071 0.764009 -0.878884
 H 1.724900 0.235289 -1.846848
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 H -0.485608 -1.616314 0.379829
 H 2.691355 -1.482783 -0.703739
 H -2.530655 1.559541 0.538409
 H -0.605581 2.295171 0.337747
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 H 2.015491 0.242319 1.744685
 H 2.298955 -1.732693 0.764106
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 H -2.444053 -1.295594 0.921649
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o.10h2o, E= -839.807674
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 O -2.334578 0.666667 0.134214
 O -0.388997 0.141103 -1.572097
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 O 2.240157 -0.434175 -1.678994
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 H 2.269888 0.224828 1.479427
 H -0.827430 3.149536 0.127004
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 H -1.315216 -0.150514 1.489766
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 H 1.236800 2.437844 -0.547243
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 H 2.616412 0.719196 -0.638693
 H 3.627535 1.755672 -0.005492

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 H -0.655216 -1.605873 -2.203087
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 H 2.285388 -1.374694 0.601089
 H 1.618238 -1.569813 -0.768189
 H 0.034106 1.606240 1.257282
 H -0.400295 0.416837 2.142526
 H 2.890308 0.741420 0.587028
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 H 1.607729 1.883732 -0.792565
 H 0.484638 0.325275 -1.533021
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 H -1.222046 -1.739003 1.489179
 H 1.711174 -0.004842 -2.406391
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 H -1.438394 2.921983 -0.183356

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 o 0.10h2o, E= -839.806570
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 O -1.758820 0.985004 -1.604715
 O 0.664188 -2.770889 0.360940
 O -1.525970 -2.193485 -1.190276
 O -3.382541 -0.539042 0.100336
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 H 1.809208 -0.531109 -1.619473
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 H 1.241814 1.442358 -1.592143
 H -0.011209 0.674036 -2.111585
 H -2.449514 0.474868 -1.125419
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H 0.597369 -2.165306 1.129520
 H 1.350913 -2.366621 -0.202149
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 H 0.497689 -1.182885 3.273502
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H	2.785869	0.366903	-1.592050	H	-0.549315	0.677498	1.423739
H	2.493649	1.672762	-0.846715	H	-0.268040	1.001091	-0.078158
H	0.535714	-2.601582	0.265086	H	1.652841	1.149964	1.419424
H	1.216463	-1.360424	0.863734	H	3.049311	0.658307	0.935552
O	-1.393405	-0.672445	2.162228	H	0.511805	-1.572839	1.980540
H	-0.483746	-0.325749	2.236769	H	1.907315	-0.917690	1.906065
H	-1.326230	-1.371347	1.481609	H	1.579593	-1.802745	-0.025928
	34			H	1.102100	-1.010689	-1.292742
O	0.11h2o,	E=	-916.266390	H	3.212279	-0.559706	-0.885775
O	-0.193190	-0.245720	1.518625	H	3.202947	0.946002	-1.173278
O	-2.351990	1.478182	1.148559	H	1.526947	2.426231	-0.675259
O	2.264853	-0.700660	2.542075	H	1.033710	1.354283	-1.646589
O	3.559913	0.430708	0.325323	H	-2.081273	0.518199	-1.312891
O	1.057837	1.779007	0.134827	O	-3.016523	0.638520	-1.024914
O	2.587925	-1.178649	-1.739556	H	-3.002803	1.454810	-0.493749
O	0.324478	-2.236810	-0.373786	O	-2.384776	2.996451	0.499625
O	0.732609	0.754268	-2.345994	H	-1.554761	2.515941	0.730791
O	-3.387969	-0.526148	-0.354194	H	-2.117186	3.646792	-0.157281
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H	-1.877018	-1.393404	-2.864805	O	-0.781409	-0.313183	1.243564
H	-3.139380	-1.220771	0.294918	O	1.479695	-0.835145	2.131645
H	-3.154483	0.310092	0.120475	O	3.150900	0.849270	1.084651
H	-1.570187	0.930948	1.391230	O	-0.632770	-1.985799	-0.990535
H	-1.985412	2.299243	0.768517	O	3.110484	-0.555434	-1.106419
H	-0.310775	-1.847339	-1.006903	O	0.646388	0.077142	-2.311394
H	0.297340	-1.635555	0.399175	O	1.770765	3.124888	0.062454
H	1.937851	-1.713862	-1.243874	O	-0.522364	1.782991	-0.412245
H	3.072426	-0.675159	-1.048362	O	-3.342357	-1.223835	-0.858199
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H	1.371491	-0.604062	2.115535	H	-3.464993	-1.068926	0.092275
H	-1.474179	-1.490534	1.625722	H	-1.471268	1.922568	-0.629102
O	-2.105585	-2.227096	1.429199	H	-0.552338	1.068854	0.277940
H	-1.557761	-2.822170	0.900522	H	-0.800984	-0.968203	0.512281
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O 1.710235 -2.697934 0.227240
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O -2.068003 1.117061 0.279152
O -0.134069 -0.226121 -1.068073
O 1.091480 2.179790 -1.084059
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O 2.170455 -3.269442 0.471645
O 0.443323 -1.336753 1.291404
O -2.220423 -1.237973 1.852404
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H -1.578938 -1.454272 -0.976816
H -3.105224 -1.320999 -1.112346
H -3.834216 0.702148 -2.196595
H -3.477830 0.760943 -0.700503
H -1.380012 0.669316 -0.280973
H -1.659718 1.964162 0.564018
H 1.528485 -0.893100 -1.439672
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H 1.564619 -2.659856 0.953313
H 1.585370 -3.921768 0.073409
H -0.452914 -1.391448 1.704132
H 0.234952 -1.102377 0.353053
H 0.099121 3.128042 0.172280
H 0.059853 2.820645 1.657518
H -2.279082 -0.304528 1.571369
H -2.436682 -1.703854 1.017187
H 0.631911 1.328637 -1.295406
H 2.051068 1.986806 -1.149208
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O 2.194920 -1.436836 -0.416076
O -1.314356 -2.416792 1.340716
O -0.024217 -3.127376 -1.097922
O 2.164214 1.723210 1.035123
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O -0.925433 2.351533 0.646391
O -0.438084 1.893966 -2.095561
O -3.636325 1.661377 0.955126
O -3.459205 -0.959408 0.265257
H 1.501697 -1.050675 0.180733
H 3.024052 -1.254904 0.059376
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O -1.151113 -2.436245 -0.768129
O 1.067872 -1.796986 -1.820310
O 2.907673 -1.306350 0.035274
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O -1.108747 -2.061893 1.893376
O 2.824577 1.526278 -0.328303
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H -0.585636 1.674781 -2.075392
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H -2.001766 1.153030 -1.680496
H 1.188615 -2.375882 -2.577686
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O 1.101411 -2.136424 1.519666
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O 1.336479 2.215510 1.434594
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 O -1.755027 -2.134569 -0.725169
 O -1.432855 -2.175988 2.017996
 O -3.892289 -0.513506 -1.542461
 O -2.963717 1.767524 -0.449797
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 H 3.166122 0.750027 0.437468
 H 0.830795 -1.726301 0.371886
 H 1.790786 -1.153058 1.390348
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 H -0.077802 2.798647 -0.198581
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 H 2.694472 -2.165297 -0.811523
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 H 1.385844 0.684816 -1.010041
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19
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19
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19

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H -0.138781 -1.004230 0.369691
H 0.571142 1.845388 0.792794
H -0.439528 0.905030 1.463358
H -1.250080 1.542606 -0.439006
H -0.709289 0.392738 -1.274960
H 2.006988 -1.278107 -0.341948
H -2.443918 -1.150734 0.537779
H -2.753226 -0.232352 -0.614528
H 1.476732 0.741768 -0.839245
H 2.633585 0.827251 0.117819

19

oh2.6h2o, E= -533.962728
O -1.263786 0.366952 -1.291750
O -2.054633 -1.939783 0.119188
O -1.834463 0.621696 1.436108
O 0.141972 2.444354 -0.842095
O 3.421225 -0.787231 0.009982
O 0.668663 -1.294073 -0.638805
O 1.086692 0.773881 1.261051
H -1.935962 -1.225938 -0.545486
H -2.104974 -1.401724 0.926343
H 0.032460 -0.658156 -1.081889
H 0.052716 -1.924625 -0.233615
H -0.466324 1.624837 -1.080279

H 3.106925 -0.097861 0.610005
H 2.588816 -1.113330 -0.373465
H -1.817257 0.681476 0.456816
H -0.895931 0.723843 1.669644
H 0.906709 1.491339 0.620228
H 0.951013 -0.032224 0.723037
H -1.743553 0.445977 -2.120759

19

oh2.6h2o, E= -533.962717
O 0.911053 -0.682064 -1.230725
O 0.932663 0.291005 1.458617
O -0.504601 -2.209790 0.771850
O -2.722504 -0.771258 -0.120339
O -1.146685 0.958314 -1.230587
O -0.830813 2.428517 0.783930
O 3.511529 0.074361 -0.324402
H 1.023173 0.063208 0.513417
H 0.335617 1.065590 1.438119
H 2.718819 -0.220674 -0.810875
H 3.146398 0.323674 0.533541
H -0.087730 -1.507887 1.299048
H -1.353188 -1.811278 0.478771
H 0.147514 -0.042502 -1.369881
H -1.453303 1.360797 -2.047390
H -3.058311 -0.277354 0.633948
H -2.155835 -0.093806 -0.627801
H -0.973762 1.880742 -0.112907
H 0.505476 -1.453186 -0.794748

19

oh2.6h2o, E= -533.962661
O -0.940746 -0.264723 -1.130549
O -2.631472 -1.896489 0.048280
O -1.453696 2.188197 -0.241957
O 2.893133 -1.230737 -0.394391
O 1.414824 1.239373 -0.837286
O 0.329607 1.245906 1.811489
O 0.273716 -1.431404 0.869743
H -0.936431 -0.487276 -2.065546
H 2.155092 -1.552373 0.145914
H 2.587046 -0.343931 -0.655640
H -1.415983 1.273341 -0.641618
H -0.647468 2.588526 -0.590282
H 0.625629 0.691999 -1.055777
H 1.309508 1.377387 0.123168
H -2.067564 -1.196844 -0.443395
H -0.070400 -1.049623 0.006771
H -0.477473 -1.958968 1.167720
H -0.449083 1.579214 1.326378
H 0.304199 0.277557 1.679675

19

oh2.6h2o, E= -533.961780
O 0.218238 0.438825 1.341638
O 1.466895 1.609745 -0.713008
O -1.652164 1.673360 -0.190720
O 1.220997 -1.164862 -1.571351
O 2.810842 -0.563528 0.790212
O -0.821929 -1.643778 0.395421
O -3.415554 -0.573628 -0.152317
H -1.031669 1.263371 0.467196

H -1.077460 1.858825 -0.941936
 H -2.918660 0.259264 -0.260446
 H -2.741394 -1.194095 0.165662
 H 0.997715 1.336099 0.118266
 H 2.363520 1.299439 -0.525743
 H 1.961689 -0.250256 1.169515
 H 2.510990 -1.011042 -0.019701
 H -0.411129 -0.805610 0.892078
 H 0.484046 -1.479124 -1.013517
 H 1.166620 -0.194545 -1.503240
 H 0.077144 0.708599 2.252862

19

oh2.6h2o, E= -533.961474

O -1.785704 -0.038295 -0.258433
 O 0.255972 1.135351 0.713049
 O 0.711412 0.385318 -1.933167
 O 2.930322 1.082046 0.010040
 O 1.578150 -1.003465 1.610641
 O -4.341599 0.442870 0.462975
 O 0.211691 -2.099001 -0.569834
 H -1.597473 0.143636 -1.188063
 H -3.387038 0.253557 0.214914
 H -1.015607 0.459756 0.229454
 H 0.030695 1.934183 1.197124
 H -0.632469 -1.657770 -0.369995
 H 0.761677 -1.885288 0.215754
 H 2.400974 -0.671858 1.221222
 H 0.986387 -0.211897 1.480859
 H 0.548755 0.870519 -1.096192
 H 0.667851 -0.546688 -1.642192
 H 2.733585 0.811150 -0.897204
 H 2.020714 1.262109 0.352149

19

oh2.6h2o, E= -533.960430

O 2.387289 -0.111670 -0.114109
 O 0.500421 -0.943681 1.824262
 O -0.906725 0.861468 0.152899
 O -3.568400 1.144888 -0.028683
 O -0.701329 -2.595570 -0.164242
 O 0.380711 -0.677564 -1.511486
 O 1.459094 2.601227 0.019843
 H 3.137473 -0.668117 -0.337628
 H 1.998694 1.793901 -0.020284
 H 0.558327 2.239434 0.073729
 H -0.567198 0.390365 0.940565
 H 0.125987 -1.659744 1.272045
 H 1.288453 -0.658213 1.320333
 H -1.599414 -2.263593 -0.063476
 H -0.277268 -1.935302 -0.808190
 H 0.350420 -0.526772 -2.458413
 H -0.482767 0.341686 -0.605051
 H -2.567395 1.060816 0.048388
 H 1.626187 -0.347245 -0.789896

19

oh2.6h2o, E= -533.960021

O -1.858601 -1.405908 -0.143919
 O 0.205402 -0.797750 1.307977
 O -0.337121 1.706475 0.733312
 O 1.701142 2.543393 -0.691178

O 0.828843 -2.567094 -0.730685
 O 2.519654 -0.266183 -0.093423
 O -2.781044 1.045816 -0.614751
 H -2.459730 0.101997 -0.560936
 H -3.451938 1.100444 0.072521
 H -1.169217 1.633704 0.229732
 H -0.123026 0.760823 1.023519
 H 0.254665 -1.001832 2.245128
 H -1.148962 -1.176327 0.544555
 H 0.613759 -2.157986 0.137769
 H 1.525563 -1.960552 -1.025190
 H 1.760619 -0.421199 0.520168
 H 2.411019 0.653787 -0.379472
 H 0.886655 2.266729 -0.140697
 H -1.325604 -1.869591 -0.805753

19

oh2.6h2o, E= -533.959824

O -1.895180 -0.775908 -0.117485
 O 0.193468 -0.636130 1.813511
 O 1.136403 1.717271 0.566052
 O 3.739335 0.268574 -0.205940
 O 1.662155 -1.361776 -0.507011
 O -0.097764 0.376649 -1.364081
 O -4.355323 0.437081 -0.063936
 H -1.862530 -1.690782 -0.412345
 H -3.501210 -0.053261 -0.124164
 H -4.122386 1.217107 0.448323
 H -1.178844 -0.252164 -0.724815
 H -0.270445 0.718362 -2.244010
 H -0.641807 -0.706668 1.309859
 H 0.521365 0.258493 1.578969
 H 2.059656 1.478460 0.397998
 H 0.646959 1.350183 -0.226317
 H 1.032818 -0.759513 -1.010347
 H 1.256506 -1.353039 0.384368
 H 2.995163 -0.413278 -0.346391

19

oh2.6h2o, E= -533.959099

O 0.467712 0.542493 -1.350872
 O -0.479026 1.214087 1.028331
 O 2.093938 -1.206161 -0.369680
 O -3.277572 0.771728 0.142304
 O -1.550412 -1.223511 -0.922732
 O 2.398169 1.629766 0.271350
 O 0.255201 -1.924483 1.395237
 H -0.832421 -0.591287 -1.196761
 H -1.173660 -1.652192 -0.140703
 H -2.840523 0.016030 -0.298204
 H -2.518477 1.252681 0.504556
 H 1.485848 -0.642767 -0.948736
 H 2.621018 -0.510905 0.055531
 H 1.796066 1.390535 -0.475947
 H 1.755807 1.707882 0.990494
 H -0.217210 1.056334 0.073824
 H -0.683266 0.330546 1.357577
 H 1.008136 -1.729923 0.740276
 H 0.334599 0.941720 -2.213410

19

oh2.6h2o, E= -533.958721

O 2.968331 1.627495 -0.001732
 O 2.439256 -0.969143 -0.245037
 O 0.021151 -1.351806 1.529399
 O -2.497285 -1.114257 -0.259714
 O -2.820272 1.742343 0.006680
 O 0.000686 1.249336 0.266241
 O 0.043742 -0.913223 -1.212625
 H 2.831673 0.627203 -0.121060
 H 2.173146 -1.273427 0.633392
 H 1.543416 -0.981902 -0.741928
 H 0.001365 -0.380117 1.446226
 H -2.239734 -1.276024 0.656298
 H -1.614691 -1.056406 -0.716361
 H -1.862771 1.838071 0.143470
 H -2.904265 0.783841 -0.147722
 H 0.881391 1.647269 0.204939
 H -0.013759 0.543686 -0.449054
 H -0.017081 -1.028905 -2.163845
 H -0.023556 -1.609237 0.589943

22

oh2.7h2o, E= -610.430495

O -0.000296 -1.111203 -1.407808
 O 0.000663 1.389979 -1.630650
 O 2.451522 -1.155156 -0.244019
 O -2.452286 -1.154084 -0.244296
 O 2.139222 1.582279 0.163326
 O -2.138386 1.583261 0.163255
 O -0.000576 -1.802946 1.359986
 O 0.000183 0.923026 1.904827
 H -0.000255 -1.649486 -2.204461
 H 1.623853 -1.165098 -0.795874
 H 2.129702 -1.526584 0.589871
 H 0.000265 0.317967 -1.613481
 H -1.624536 -1.164370 -0.796020
 H -2.130773 -1.525666 0.589642
 H -0.000483 -1.738973 0.385875
 H -0.000267 -0.861057 1.649051
 H -2.416501 0.647488 0.049307
 H -1.573108 1.739516 -0.615049
 H -0.776246 1.249928 1.405083
 H 0.776677 1.249652 1.405015
 H 2.416672 0.646291 0.049404
 H 1.574637 1.739157 -0.615343

22

oh2.7h2o, E= -610.429141

O 2.113024 1.610768 -0.088473
 O 0.006673 1.121333 -1.807083
 O 0.190549 -1.675276 -1.375045
 O 2.533492 -1.164210 0.231209
 O 0.050001 1.170383 1.757206
 O -2.107599 1.627625 -0.018651
 O -2.551766 -1.139734 0.029222
 O -0.188231 -1.278528 1.262953
 H 1.627484 1.684716 0.750265
 H 1.401715 1.528122 -0.767995
 H -0.782703 1.397615 -1.295159
 H 0.005042 0.142815 -1.758738
 H -0.003743 -1.651295 -0.403231
 H 1.161033 -1.677991 -1.350699
 H 2.583661 -0.199030 0.075708

H 1.699959 -1.252943 0.732718
 H -2.440644 0.705337 -0.018591
 H -1.487039 1.641265 0.734814
 H -2.234922 -1.433619 -0.833104
 H -1.743396 -1.243028 0.608921
 H -0.121308 -1.934903 1.961381
 H -0.034276 0.114056 1.633005

22

oh2.7h2o, E= -610.428299

O 0.423098 -1.396250 -1.049593
 O 0.402068 1.031568 -1.792890
 O 2.728769 -1.178033 0.087138
 O -2.313153 -1.211825 -0.539177
 O 1.967350 1.559750 0.479310
 O -2.011417 1.566398 -0.431069
 O -0.592913 -1.574443 1.673014
 O -0.455960 1.206106 1.911259
 H 0.466945 -2.122486 -1.678813
 H 1.798918 -1.323475 -0.345803
 H 0.409669 0.018177 -1.582497
 H 0.647016 1.131310 -2.716070
 H -1.392915 -1.285744 -0.884273
 H -2.146524 -1.420236 0.398257
 H -0.108687 -1.659391 0.831517
 H -0.528514 -0.615510 1.881701
 H -2.309851 0.632370 -0.476193
 H -1.222971 1.561503 -1.005006
 H -1.071901 1.435232 1.184149
 H 0.429831 1.404631 1.545143
 H 2.357027 0.665842 0.516429
 H 1.489223 1.551606 -0.372474

22

oh2.7h2o, E= -610.427913

O 0.229056 -1.410441 -1.441044
 O -1.685253 -1.460227 0.199564
 O 0.703834 1.356041 -1.658056
 O 2.356050 -1.511414 0.392421
 O -3.391305 0.385935 -0.051959
 O 0.124633 -0.294670 1.798817
 O -1.016690 1.923954 0.429620
 O 2.520471 1.303083 0.399032
 H -0.001037 -1.901751 -2.233639
 H -0.588758 -1.476694 -0.794604
 H -1.990687 -2.329548 0.472576
 H 0.534469 0.392808 -1.698374
 H 0.008669 1.684612 -1.044486
 H 1.707617 -1.609053 -0.331943
 H 2.657101 -0.584627 0.315808
 H -0.599842 -0.783488 1.319508
 H 0.928594 -0.766614 1.512335
 H -0.575796 1.258555 0.995647
 H -1.894456 1.535614 0.244670
 H 1.988220 1.414438 -0.425874
 H 1.841604 1.262878 1.085590
 H -2.742075 -0.435215 0.035632

22

oh2.7h2o, E= -610.427423

O 0.155527 -0.268291 -1.607748
 O -1.361413 -1.495210 -0.099480

O	2.441435	1.001330	-0.807151	H	-0.186672	2.093346	0.267688
O	-1.263634	1.815619	-0.554178	H	-1.901051	-0.338654	1.074004
O	-3.558610	-0.067344	0.121664	H	-2.098270	1.013870	-0.743598
O	2.048511	-1.821741	-0.153661	H	-1.713801	-0.470850	-1.077024
O	0.825437	1.850819	1.336638	H	-0.300280	0.772577	1.885539
O	0.484913	-0.836503	1.991072	H	1.175229	1.004661	1.438751
H	0.012404	-0.392367	-2.550114	H	-0.779528	-1.267349	1.580777
H	1.607386	0.678089	-1.228329	H	1.246347	-1.685876	0.749896
H	2.799312	0.166919	-0.465178				
H	1.426561	-1.425995	-0.796671				
H	1.647591	-1.571589	0.704523				
H	-0.710419	-1.006546	-0.811355				
H	-1.212107	-2.442159	-0.165921				
H	-0.756080	1.113098	-1.034445				
H	-2.090100	1.384128	-0.291064				
H	0.016971	1.977129	0.798023				
H	1.515716	1.692968	0.658956				
H	0.622883	0.132911	1.888471				
H	-0.277164	-1.027432	1.414860				
H	-2.780277	-0.708579	0.060994				
22							
oh2.7h2o,	E=	-610.426552					
O	0.209398	-1.240666	1.709642				
O	-1.990171	-1.389450	0.075591				
O	-0.268015	-0.809425	-1.993472				
O	1.960151	-1.574035	-0.479527				
O	2.617105	1.168538	-0.384405				
O	0.775563	1.147250	1.470352				
O	-0.456912	1.719255	-0.803893				
O	-3.179606	0.983234	0.153053				
H	-1.299526	-1.424544	0.774853				
H	-1.457127	-1.315851	-0.752636				
H	0.437201	-0.189810	1.704380				
H	0.666959	1.774077	2.188912				
H	1.414702	-1.593547	0.332903				
H	2.353668	-0.675993	-0.474952				
H	2.033533	1.499813	-1.077647				
H	2.034314	1.236543	0.431432				
H	0.553250	-1.181317	-1.604718				
H	-0.269605	0.126052	-1.692325				
H	-0.052264	1.555623	0.099631				
H	-1.413884	1.686224	-0.648266				
H	-2.766887	0.052583	0.161265				
H	0.425552	-1.587458	2.578437				
22							
oh2.7h2o,	E=	-610.425636					
O	-0.459318	-1.306593	-1.619835				
O	0.454017	-2.239913	0.675187				
O	2.399418	-0.052366	0.541831				
O	1.345952	0.429333	-1.777703				
O	-0.521955	2.337546	-0.663145				
O	0.359059	1.488707	1.673455				
O	-1.390691	-0.557178	1.887464				
O	-2.407719	0.106150	-0.614095				
H	-0.630114	-1.880266	-2.370559				
H	0.095384	-2.007214	-0.235335				
H	3.355243	0.029144	0.495463				
H	2.045561	0.140800	-0.392339				
H	0.600842	-0.313727	-1.809202				
H	0.861010	1.264052	-1.689340				
22							
oh2.7h2o,	E=	-610.423057					
O	1.840638	-0.223236	0.104745				

O 4.498119 0.086953 -0.123016
 O 0.031362 0.509322 2.097233
 O -0.770958 2.317818 0.156973
 O -2.794662 0.514055 -0.875879
 O -0.128516 0.397880 -1.614619
 O -1.881298 -1.406792 1.125865
 O -0.218456 -2.061331 -0.810398
 H 1.235029 0.108283 -0.616837
 H 1.361111 0.009406 0.930258
 H -0.651832 -0.165750 1.939888
 H -0.255721 1.265510 1.534339
 H -0.381636 1.741561 -0.555691
 H -1.709793 2.094857 0.053695
 H -1.905885 0.448585 -1.303268
 H -2.731015 -0.126017 -0.149729
 H -1.269270 -1.741911 0.401541
 H -2.294257 -2.183025 1.513204
 H -0.263280 -1.163853 -1.287960
 H 0.656315 -1.983577 -0.399093
 H 3.501196 -0.001897 -0.026831
 H 0.099199 0.620479 -2.520747

22

oh2.7h2o, E= -610.422801

O 0.715955 -1.403694 -0.774898
 O 0.602448 -0.315703 1.701127
 O 0.015473 0.997682 -1.752822
 O 3.166028 -0.570891 0.061411
 O -1.891942 -1.726443 -0.733926
 O -2.144828 -0.219050 1.565065
 O 1.728535 1.878749 0.271851
 O -2.450542 1.695707 -0.269521
 H 0.991472 -2.200896 -1.236850
 H 0.275241 0.068127 -1.508837
 H -0.848803 1.163094 -1.342301
 H 2.316869 -0.878134 -0.360927
 H 2.972964 -0.701227 0.997898
 H 0.634724 -0.881152 0.889837
 H 0.915040 0.552514 1.371838
 H -0.880861 -1.649223 -0.736447
 H -2.170275 -1.095220 -1.405774
 H -2.182455 -0.907814 0.863847
 H -1.187344 -0.209967 1.802792
 H -2.347295 1.059404 0.514012
 H 2.447668 1.241904 0.104246
 H 1.134044 1.747725 -0.499629

22

oh2.7h2o, E= -610.422528

O 0.210221 0.855702 -1.220389
 O 2.149015 -0.356559 0.106817
 O -0.398080 -1.619833 -1.027510
 O -0.572427 2.029879 1.063034
 O 4.819107 -0.016326 -0.059706
 O -0.337739 -0.645265 1.772883
 O -2.851012 -1.449383 0.301374
 O -2.572523 1.213982 -0.827772
 H -1.645534 1.082763 -1.125762
 H -2.843610 0.338910 -0.497124
 H -1.494939 2.031555 0.757007
 H -0.113804 1.779320 0.219160
 H -0.196558 -0.643642 -1.256628

H 0.476079 -2.000928 -0.887189
 H 1.507929 0.196063 -0.439116
 H 1.715499 -0.443396 0.967788
 H -0.435366 0.330107 1.671902
 H -0.338759 -0.973681 0.857597
 H -2.420278 -1.225557 1.139275
 H -2.093211 -1.724251 -0.251217
 H 3.824529 -0.121606 0.012899
 H 0.485530 1.276763 -2.038436

22

oh2.7h2o, E= -610.422257

O 0.261275 -1.763433 -0.376987
 O 2.773583 -0.719494 0.360665
 O 2.083551 1.932832 -0.655509
 O 0.466841 -0.854624 2.083245
 O 0.128261 0.332968 -1.806445
 O -0.502018 1.325507 0.783646
 O -3.169522 1.016035 0.910245
 O -2.338040 -1.072942 -1.148334
 H -1.496760 -1.425069 -0.770600
 H -2.728516 -0.527597 -0.449490
 H -0.788884 0.238797 -2.100560
 H 0.291399 -0.569455 -1.345010
 H 0.270637 -1.378772 1.252062
 H 1.423292 -0.721822 1.975506
 H 1.980524 -1.165392 -0.015609
 H 2.725473 0.187203 0.009820
 H -0.339011 0.997293 -0.126592
 H -0.153943 0.598610 1.365139
 H -2.178612 1.209304 0.923826
 H 1.480818 1.501488 -1.292582
 H 1.486251 2.135200 0.078469
 H 0.395877 -2.654575 -0.708585

22

oh2.7h2o, E= -610.422052

O -0.000627 -0.907215 -1.422297
 O 0.000467 1.282693 -1.609259
 O 2.486582 -1.240504 -0.279512
 O -2.487855 -1.238823 -0.279329
 O 2.069268 1.522655 0.192748
 O -2.067660 1.524005 0.193174
 O -0.000769 -1.741148 1.347124
 O 0.000695 0.923349 2.015896
 H -0.000119 -1.102586 -2.366781
 H 1.673188 -1.100010 -0.822657
 H 2.116710 -1.605253 0.537280
 H -0.000785 1.187306 -2.569092
 H -1.674549 -1.098998 -0.822770
 H -2.117981 -1.603731 0.537391
 H -0.000752 -1.612686 0.385561
 H -0.000382 -0.814902 1.694527
 H -2.454584 0.631271 0.121384
 H -1.407179 1.522021 -0.534395
 H -0.773654 1.223635 1.492658
 H 0.775126 1.222987 1.492415
 H 2.455285 0.629520 0.120982
 H 1.408866 1.521332 -0.534852

22

oh2.7h2o, E= -610.421962

O	1.093282	-1.053764	-1.000560	H	1.483959	0.696920	-1.249846
O	-0.521286	1.120904	-1.084933	H	2.745565	0.675386	-0.343459
O	-0.909898	-3.034550	-0.194418	H	2.549237	-1.372069	0.680899
O	-2.100097	-0.551025	0.065073	H	0.700187	-1.105718	-0.489609
O	0.250786	-0.952994	1.695616	H	0.289526	-2.297891	0.440157
O	-2.538396	2.437801	0.021337	H	-1.009044	0.780803	-1.524704
O	1.234837	1.806531	0.894419	H	-2.247481	0.962532	-0.615707
O	3.475114	0.452059	-0.288562	H	-1.908607	-0.012846	1.380882
H	0.804684	-0.985413	0.890590	H	-3.477758	-0.054495	1.518276
H	-0.627849	-0.734985	1.332754	H	-0.181218	1.173593	1.596651
H	-1.561426	-2.307032	-0.183570	H	0.134554	-0.352883	1.542557
H	-1.526932	0.038269	-0.527116	H	-1.124831	-1.657488	-1.207811
H	0.529651	-0.241991	-1.119817	H	-2.217090	-1.746768	-0.144405
H	-0.470764	1.429352	-1.993680	H	0.971178	2.258788	0.127081
H	0.979052	1.087636	1.490613	H	-0.549336	2.336773	-0.106162
H	0.635190	1.681450	0.119007	H	0.463744	-0.727622	-2.543181
H	0.492265	-1.813651	-1.067830				
H	-0.431726	-2.885057	0.633423				
H	-1.676844	2.058141	-0.365300				
H	-2.755906	0.065802	0.411215				
H	2.894269	-0.238910	-0.640063				
H	2.841608	1.046711	0.156003				
25							
oh2.8h2o,	E=	-686.888466					
O	-0.850830	1.457356	-0.535049				
O	1.411057	3.079365	-0.110443				
O	2.396782	0.625870	-0.420591				
O	0.289331	-0.674621	-1.586636				
O	-1.945606	-1.712755	-0.412499				
O	-3.425437	0.769012	0.093066				
O	-0.978963	-0.200591	1.726318				
O	1.744124	-0.967078	1.788009				
O	1.507886	-2.681995	-0.496521				
H	-0.411694	0.696562	-1.024542				
H	-0.185727	2.169682	-0.468308				
H	1.423156	3.219015	0.841557				
H	1.883312	2.206891	-0.239345				
H	1.706334	0.175973	-0.969363				
H	2.322335	0.155671	0.438001				
H	-1.171152	-1.393662	-0.942604				
H	-2.620611	-1.020842	-0.508261				
H	-3.151095	0.521344	0.985842				
H	-2.616582	1.201491	-0.254356				
H	-0.847679	0.509701	1.063739				
H	-1.300246	-0.934739	1.158820				
H	1.691223	-1.717100	1.164612				
H	0.809374	-0.702452	1.917192				
H	1.004399	-1.921975	-0.981301				
H	0.277898	-0.722076	-2.546910				
25							
oh2.8h2o,	E=	-686.887341					
O	2.189589	1.278100	-0.858769				
O	3.496863	-1.035162	0.726890				
O	0.931600	-1.574474	0.416967				
O	0.207984	-0.397444	-1.677703				
O	-1.682773	1.453425	-1.234045				
O	-2.765583	-0.210877	0.892944				
O	-0.432046	0.303563	2.000519				
O	0.141385	2.548491	0.562635				
O	-1.664843	-2.310249	-0.712139				

H 1.531626 -1.210417 -1.272112
 H -2.176530 -0.683505 1.254883
 H -2.320565 0.825037 1.414575
 H -2.231036 1.421698 -0.719235
 H -1.016004 2.035995 -0.033289
 H 0.653448 0.684377 0.626080
 H 0.713315 0.668375 -0.889433
 H 2.105934 -1.185556 0.922078
 H 3.225368 -0.417245 0.204925
 H 2.449125 1.619830 -0.068845

25

oh2.8h2o, E= -686.885738

O -1.340511 -1.586096 0.224592
 O -2.285953 0.593017 1.877472
 O 0.399350 -0.254339 1.617473
 O 0.780129 -1.432978 -1.498092
 O -2.979766 -0.536448 -1.433126
 O -1.950390 1.986634 -0.579555
 O 2.803770 -1.279598 0.564694
 O 3.493088 1.368617 -0.336958
 O 0.800901 1.171192 -0.700892
 H -1.540101 -2.494454 0.468130
 H -2.324217 -1.022733 -0.787233
 H -0.214700 -0.881307 1.107463
 H -0.249701 0.243887 2.141770
 H -0.021871 -1.611117 -0.943607
 H 1.534192 -1.596999 -0.900285
 H -2.198115 -0.255789 1.401296
 H -2.234626 1.243245 1.147544
 H -2.364496 1.217067 -1.018450
 H -0.994816 1.857229 -0.726987
 H 0.661980 0.801045 0.203639
 H 0.765243 0.340684 -1.238389
 H 2.094886 -0.968095 1.155918
 H 3.217301 -0.456977 0.244342
 H 2.535769 1.418108 -0.583573
 H 3.568334 1.926200 0.443546

25

oh2.8h2o, E= -686.885612

O -0.219660 -1.488958 0.961450
 O 1.989576 -1.625849 -0.352379
 O 0.372533 0.812652 1.832159
 O 3.086673 0.621352 1.086683
 O -1.584610 -1.469816 -1.434032
 O -0.803528 1.207776 -1.886705
 O -1.928583 2.004224 0.498692
 O -2.973532 -0.571978 0.898392
 O 1.980619 0.889120 -1.578824
 H -2.079383 -0.920124 1.078295
 H -2.805916 0.386922 0.778841
 H -2.407124 -1.220186 -0.978106
 H -0.999529 -1.616996 -0.656606
 H 2.399469 1.238414 -0.774892
 H 1.952672 -0.065808 -1.372502
 H 1.105715 -1.625041 0.165847
 H 2.021927 -2.451289 -0.842760
 H -1.053164 0.260165 -1.862705
 H 0.172612 1.213359 -1.817926
 H -1.550736 1.827224 -0.395614
 H -1.192021 1.809252 1.101419

H 2.992771 -0.266798 0.704820
 H 0.105335 -0.162246 1.513161
 H -0.252730 -2.195922 1.612972
 H 2.234198 0.760902 1.542265

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oh2.8h2o, E= -686.885214

O -0.602613 0.506775 -1.643496
 O -2.343901 -1.614534 -0.926666
 O 0.489469 -1.710443 -0.880733
 O 0.810451 1.805612 0.152580
 O -2.175251 1.988656 -0.067381
 O -2.604099 -0.246406 1.564841
 O 3.653044 1.043061 -0.350443
 O 2.769644 -1.327151 0.583629
 O 0.275563 -0.424165 1.673225
 H -0.540294 0.772299 -2.564546
 H -1.710738 1.445770 -0.764891
 H -1.436425 2.454581 0.343658
 H 0.179872 -0.827986 -1.280312
 H -0.346437 -2.206107 -0.861046
 H 0.361484 1.363994 -0.634273
 H 1.762850 1.777645 -0.027161
 H -1.914269 -0.828307 -1.325174
 H -2.575760 -1.299996 -0.030105
 H -2.596577 0.598227 1.064832
 H -1.674285 -0.347760 1.837417
 H 0.181432 -0.970372 0.867765
 H 0.452757 0.467165 1.288961
 H 3.382624 0.125162 -0.029060
 H 2.202323 -1.050694 1.324890
 H 2.092982 -1.644864 -0.055408

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oh2.8h2o, E= -686.884855

O 0.358671 -1.344813 -0.835677
 O 2.090529 0.354028 -1.607256
 O 0.906568 -0.475235 1.484475
 O 3.666610 -0.553456 0.535334
 O -1.920095 -0.242925 -1.937924
 O -1.866594 2.027779 -0.281096
 O -1.873437 0.338947 1.904077
 O -2.191989 -1.993158 0.361616
 O 0.906668 2.142003 0.244415
 H -1.293210 -1.895512 -0.006892
 H -2.251478 -1.242211 0.987985
 H -2.477199 -0.786322 -1.357055
 H -1.030466 -0.606039 -1.723826
 H 0.946120 1.451443 0.924045
 H 1.348736 1.725029 -0.519673
 H 1.354697 -0.359866 -1.404431
 H -1.913201 1.328258 -0.967630
 H -0.911885 2.214504 -0.177109
 H -2.018982 1.008456 1.195285
 H -0.912163 0.198493 1.882418
 H 3.510245 -0.312100 -0.390312
 H 0.668779 -0.916936 0.578195
 H 0.678569 -2.221539 -1.070795
 H 2.795412 -0.443523 0.954008
 H 0.890578 -1.167497 2.152070

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oh2.8h2o, E= -686.884796
 O -0.006870 -0.639665 -1.247647
 O -2.257690 -2.219641 0.326035
 O 2.242573 -0.304527 1.213235
 O 1.852684 1.174586 -0.798809
 O -1.581954 1.806139 0.941208
 O 0.534611 3.267436 -0.283288
 O -2.672133 0.232615 -1.137785
 O -0.468276 -0.580553 1.618844
 O 2.138722 -2.522882 -0.648384
 H 0.699010 0.074617 -1.244323
 H 2.577208 1.227376 -1.428055
 H 2.835292 0.115958 1.841335
 H 2.160707 0.337395 0.398123
 H 0.510256 -0.513863 1.658501
 H -0.820226 0.337932 1.511718
 H 1.409583 -2.044034 -1.077169
 H 2.359536 -1.934672 0.092095
 H -2.077026 1.412275 0.192569
 H -0.898963 2.381047 0.537649
 H -1.771136 0.055412 -1.474747
 H -2.841369 -0.574007 -0.617197
 H 1.126357 2.435821 -0.530955
 H -1.671586 -2.543514 -0.367865
 H -1.646109 -1.753328 0.937757
 H -0.204879 -0.722464 -0.296704

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oh2.8h2o, E= -686.883891
 O -2.641126 0.912141 0.023989
 O -1.953779 -1.576725 -0.219351
 O -0.136011 -1.376271 2.011751
 O -0.582879 1.216818 1.895609
 O 1.748537 -1.688742 -0.129687
 O 3.416710 0.309968 0.028564
 O 1.208590 2.193380 0.118632
 O -0.467553 1.393605 -1.874683
 O -0.069903 -1.200316 -1.884208
 H -2.438353 -0.079498 -0.079690
 H -3.597451 0.998636 0.038960
 H 1.191557 -1.686332 0.668345
 H 1.082279 -1.530694 -0.891742
 H -1.387166 1.259617 1.341893
 H 0.125762 1.624105 1.329546
 H 2.783682 -0.496871 -0.059541
 H -0.026491 -1.623527 2.933435
 H -0.274284 -0.379600 2.000912
 H 0.672202 1.952446 -0.680331
 H -1.306186 1.410606 -1.387922
 H -0.275837 0.408060 -1.978295
 H -0.055611 -1.691358 -2.709213
 H 2.004583 1.632841 0.076742
 H -1.229457 -1.506499 -0.957752
 H -1.449917 -1.762797 0.589727

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oh2.8h2o, E= -686.883626
 O -2.665516 0.946157 0.084449
 O -0.845202 1.253151 -1.810777
 O -0.294121 -1.503060 -1.873667
 O -1.752268 -1.766875 0.251362
 O 3.383155 0.591635 -0.264356

O 1.926947 -1.561852 -0.039903
 O 0.181311 -1.279818 1.828680
 O -0.433914 1.269291 1.948696
 O 1.018712 2.263395 -0.136013
 H -2.016194 1.100157 -0.665965
 H -3.426743 1.502807 -0.097893
 H 1.864133 1.779976 -0.171727
 H -2.281090 -0.952989 0.294163
 H -1.013759 -1.641732 0.967483
 H 1.315726 -1.620916 -0.793799
 H 2.835509 -0.272386 -0.156274
 H -0.540999 -2.155819 -2.533895
 H -0.902425 -1.658952 -1.070805
 H -0.158184 0.299592 1.995291
 H -1.298247 1.244955 1.509061
 H 0.568456 1.952259 0.690894
 H 0.273795 -1.780725 2.642601
 H 1.299571 -1.482961 0.766735
 H -0.098179 1.659168 -1.295707
 H -0.574199 0.331378 -1.987939

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oh2.8h2o, E= -686.883558
 O 0.291468 0.076125 1.580604
 O 2.060565 -1.458278 0.481077
 O 0.631021 1.535814 -0.582124
 O 3.484845 0.976436 -0.235317
 O -1.475516 -1.761884 1.817482
 O -1.948278 -1.689159 -1.027692
 O -2.274738 1.034695 -1.346542
 O -1.662269 2.231029 1.154824
 O 0.645559 -1.041155 -1.883325
 H -1.123955 1.474262 1.448816
 H -2.121857 1.877646 0.369126
 H -0.788416 -0.987853 1.794942
 H 0.637989 -0.077878 -1.762423
 H 1.229330 -1.342891 -1.158720
 H 1.377284 -0.891746 0.982929
 H -1.841077 -1.809788 -0.065075
 H -1.036532 -1.588629 -1.375948
 H -2.358780 0.058984 -1.243896
 H -1.319324 1.154458 -1.445412
 H 3.254658 0.070195 0.021454
 H 0.528062 0.973390 0.248406
 H 0.674566 0.466628 2.372311
 H 2.623085 1.366433 -0.453978
 H 0.137759 2.331635 -0.339568
 H 2.105960 -2.303810 0.935131

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oh2.8h2o, E= -686.882925
 O 0.170118 1.540101 -1.350468
 O 2.695391 1.615281 -0.102550
 O 2.081691 -0.225422 1.669516
 O -0.474807 -0.834759 1.400362
 O 0.236581 -1.262926 -1.043535
 O -2.557866 -1.746456 -0.324765
 O -3.974654 0.830396 -0.290288
 O -1.650470 1.461305 0.767665
 O 2.997927 -1.293274 -0.872003
 H 0.155554 0.561408 -1.394347
 H 1.052308 1.734327 -0.983379

H 3.135066	2.379802	0.278446	H -0.352858	1.451374	1.474980
H 2.432931	1.024222	0.666474	H 1.195630	1.335809	1.345920
H 1.088686	-0.408086	1.649374	H 0.407856	-0.495166	1.975621
H 2.461862	-0.901569	1.082614	H 0.459641	-1.815657	2.827564
H -1.935604	-1.431870	0.365322	H -2.353238	2.605323	0.432642
H -3.167316	-0.998974	-0.440768	H -2.351876	1.059116	0.176918
H -3.096006	1.128132	0.141377	H 1.869826	-1.568823	0.518837
H -1.035968	1.664644	0.029183	H 1.655979	-1.248472	-0.982365
H -1.262639	0.627927	1.157680			
H 2.053027	-1.422076	-1.095356			
H 3.129220	-0.337362	-0.946755			
H 0.030255	-1.188134	-0.052316			
H -0.588265	-1.634306	-1.388092			
H -0.644396	-1.472043	2.099073			
25			28		
oh2.8h2o,	E=	-686.882591	oh2.9h2o,	E=	-763.349130
O 0.968035	1.014572	1.254478	O 0.488870	2.104568	1.603710
O 2.353121	-1.388725	1.484722	O -1.927885	0.917497	1.506708
O -0.509075	-0.617311	1.544185	O -1.659024	-1.690339	1.418405
O -0.607855	1.961466	-0.719220	O 2.458811	0.148150	1.382579
O 2.365697	1.487059	-1.063482	O 1.122319	-2.222083	1.002113
O 2.162392	-1.352030	-1.377752	O 0.994848	-1.663369	-1.622231
O -2.766081	0.964196	0.834758	O 2.198491	0.476239	-1.338426
O -3.267891	-1.305267	-0.855198	O -1.573852	-1.450749	-1.420005
O -0.609997	-0.793660	-1.108426	O -2.097306	1.087767	-1.294309
H 0.692290	1.351561	2.113290	O 0.343346	2.531673	-1.164426
H 2.069268	1.388921	-0.134553	H 1.201297	1.426177	1.630509
H 1.576662	1.842375	-1.492872	H 2.731521	0.288394	0.457285
H 0.287592	-1.117191	1.795629	H 2.005601	-0.729914	1.360000
H -0.048126	1.697373	0.058213	H -0.503527	2.068225	-1.303019
H -1.508762	1.872656	-0.354395	H 0.490621	2.413735	0.671827
H 2.081652	-0.448245	1.489834	H -1.046135	1.355822	1.655437
H 2.379130	-1.585924	0.527958	H -2.139135	1.119366	0.575376
H 2.401182	-0.405498	-1.391407	H 1.108050	-2.118927	0.011020
H 1.186636	-1.323362	-1.413145	H 0.193061	-2.106697	1.265017
H -0.516864	-0.798554	-0.109453	H -1.890600	0.099040	-1.401766
H -0.582476	0.170173	-1.285953	H -2.792840	1.294064	-1.923926
H -2.036958	0.507348	1.292070	H -2.228430	-2.083502	2.084602
H -3.131822	0.271005	0.254434	H -1.749780	-0.692043	1.515808
H -2.318135	-1.180325	-1.107816	H 1.690159	-0.482561	-1.520862
H -3.238032	-2.004716	-0.194355	H 1.392193	-2.324467	-2.194998
25			H 1.031680	1.868901	-1.388107
oh2.8h2o,	E=	-686.880694	H -1.704526	-1.740250	-0.499820
O 2.348400	1.436248	0.077937	H -0.578143	-1.570188	-1.587319
O 2.368091	-1.316383	-0.273506			
O 0.334359	-0.982593	-1.925913			
O 0.307173	1.642374	-1.777082			
O -1.317594	-1.921447	-0.298267			
O -3.272530	-0.349095	-0.073122			
O -1.767857	1.850559	0.328000			
O 0.435087	1.145440	1.961283			
O 0.424805	-1.497421	1.921964			
H 2.529571	0.475086	-0.045465			
H -0.648751	-1.564126	-1.040805			
H -0.788252	-1.927067	0.519284			
H 1.720089	1.636286	-0.656084			
H -0.434826	1.796968	-1.173678			
H -2.468146	-1.043166	-0.186380			
H 0.380006	-1.403619	-2.788194			
H 0.299879	0.644674	-1.929144			

H 1.847114 1.840775 -0.088128	H 1.577829 -1.675380 -2.118196
H 2.030045 -1.527506 0.066571	H 3.038864 -1.245546 0.915078
H 2.844239 -0.242637 0.253595	H -0.420598 -1.553647 1.804667
H 0.528439 -0.984185 -1.560811	H -1.867876 -1.037748 1.595190
H 0.389048 3.380694 1.275856	H -2.553267 -1.167797 -0.544257
H -0.130949 1.885829 1.349145	H -2.928482 0.148203 0.075810
H 0.648152 -2.985603 -0.884894	O 0.968523 -2.389217 0.848288
H 0.737289 -0.445613 -3.059285	H 0.981514 -1.997665 -0.119894
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oh2.9h2o, E= -763.347814	oh2.9h2o, E= -763.346319
O -0.168353 2.204490 1.593308	O -0.128508 -0.001338 -1.613396
O -2.060150 0.300422 1.584535	O 1.611785 1.577820 -0.497782
O -1.032966 -2.096451 1.518334	O -1.532087 1.219168 0.186012
O 2.267518 0.937846 1.281816	O 3.507536 -0.036238 0.609074
O 1.799451 -1.797321 1.147954	O -3.785508 -0.287211 0.461115
O 1.302232 -1.477049 -1.453493	O -0.476677 3.670792 -0.162911
O 1.868639 0.959883 -1.503533	O 0.493607 0.267755 1.815383
O -1.216047 -1.903399 -1.316110	O -1.799918 -2.024747 -0.779600
O -2.418008 0.392193 -1.198783	O 1.898837 -1.808438 -1.053667
O -0.447248 2.442748 -1.188368	O 0.232353 -2.352272 1.083416
H 0.717099 1.771089 1.618408	H -1.076299 0.754724 -0.602564
H 2.273681 1.051049 0.311042	H -0.984940 0.906973 0.943811
H 2.147138 -0.032377 1.387646	H 0.995313 0.664753 1.079822
H -1.154704 1.780496 -1.291845	H 0.408094 -0.697562 1.602305
H -0.272525 2.458919 0.650543	H -0.598821 -2.366003 0.560341
H -1.364314 1.005268 1.704200	H 0.915825 -2.361376 0.376279
H -2.369397 0.422719 0.666631	H -3.054276 0.370744 0.366427
H 1.650603 -1.752369 0.158737	H -3.673073 -0.639673 1.349747
H 0.936833 -2.035917 1.520382	H 0.981452 0.997801 -1.040404
H -1.946509 -0.501201 -1.299817	H 1.172817 2.437308 -0.410111
H -3.184772 0.365855 -1.776799	H -1.210312 -1.336974 -1.177042
H -1.437798 -1.163279 1.629507	H -2.588876 -1.539300 -0.485418
H 1.654729 -0.073634 -1.545886	H 1.206903 -1.174694 -1.362221
H 1.794950 -2.069508 -2.027519	H 2.582050 -1.264908 -0.624415
H 0.381008 1.956318 -1.391619	H 3.008560 0.700383 0.197380
H 2.525705 1.143370 -2.179395	H 3.007897 -0.220064 1.414148
H -1.307834 -2.273963 -0.422903	H -0.981343 2.807456 -0.020487
H -0.204446 -1.759720 -1.436599	H -0.282340 0.158069 -2.548752
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oh2.9h2o, E= -763.346505	oh2.9h2o, E= -763.346230
O 1.988631 1.979716 0.684172	O 0.115707 -0.045781 -1.483025
O -0.532311 1.619303 1.699929	O 1.819513 1.101959 0.091959
O -1.857887 1.716694 -0.523257	O -1.400894 1.444107 0.057456
O 3.192729 -0.525592 0.292074	O 4.035635 -0.326034 0.065580
O 1.162565 -1.195840 -1.394820	O -3.832065 0.224749 0.002242
O -1.450076 -1.048462 -2.019011	O 0.344900 3.525987 -0.130065
O -3.051877 -0.805046 0.219606	O -0.072288 0.176805 2.056590
O -1.112872 -1.005767 2.222345	O -1.956844 -1.776153 -0.996290
O 0.760822 1.473744 -1.766902	O 1.691996 -2.131993 -0.664042
H 2.522503 1.161873 0.729773	O -0.370637 -2.415319 1.205101
H 1.648984 1.961416 -0.237847	H -0.909625 0.906436 -0.641521
H -0.153502 1.581996 -1.456505	H -1.052756 1.037252 0.892877
H 0.939834 0.500320 -1.706753	H 0.749139 0.418944 1.591422
H 0.421846 1.735152 1.471477	H -0.199337 -0.782903 1.849763
H -0.651691 0.687815 2.007392	H -1.057113 -2.314031 0.509873
H -1.349752 1.714406 0.359418	H 0.452773 -2.481226 0.677200
H -2.238072 2.596204 -0.605468	H -3.022949 0.793780 0.004336
H -1.553080 -0.089352 -2.054452	H -3.868061 -0.131807 0.895791
H -0.486800 -1.172027 -1.792406	H 1.192759 0.668926 -0.585473
H 2.525764 -0.704492 -0.422428	H 1.572094 2.044385 0.099335

H -1.219136 -1.176588 -1.271307
 H -2.698905 -1.182580 -0.791038
 H 1.134948 -1.414344 -1.058112
 H 2.527081 -1.703699 -0.424081
 H 3.266860 0.324724 0.109144
 H -0.398299 2.880123 -0.014409
 H 0.323273 3.747087 -1.066199
 H 0.207069 0.138894 -2.421646

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oh2.9h2o, E= -763.346181
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 O 1.388483 1.712138 -0.472569
 O -1.682782 0.937684 0.366297
 O 3.488415 0.276996 0.494462
 O -3.878120 -0.587818 0.448880
 O -0.826773 3.486911 -0.113837
 O 0.531302 0.221886 1.857981
 O -1.617425 -2.254082 -0.679160
 O 2.017473 -1.605681 -1.164324
 O 0.564317 -2.394522 1.056008
 H -1.196283 0.563276 -0.451732
 H -1.074267 0.686306 1.100155
 H 0.945574 0.697174 1.115035
 H 0.557348 -0.740236 1.619666
 H -0.297248 -2.497269 0.599768
 H 1.188371 -2.306158 0.301561
 H -3.097843 0.053267 0.473043
 H 0.805621 1.075782 -0.993298
 H 0.834997 2.497009 -0.314444
 H -1.128368 -1.491556 -1.080150
 H -2.448922 -1.877526 -0.355426
 H 1.237901 -1.049191 -1.404098
 H 2.651634 -1.001909 -0.739308
 H 2.889490 0.967344 0.137996
 H 3.058338 0.013563 1.317407
 H -1.257499 2.633332 0.139902
 H -1.145039 3.658779 -1.005421
 H -0.460442 0.110803 -2.466482

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oh2.9h2o, E= -763.346099
 O -1.300333 -1.608786 1.818990
 O -1.714875 0.974071 1.715288
 O 0.583740 2.329656 1.258691
 O 1.429557 -1.971559 1.005559
 O 2.577401 0.361588 1.015754
 O 0.000478 2.332585 -1.434213
 O -2.394527 0.848446 -0.980184
 O -1.821316 -1.671010 -0.966055
 O 0.637532 -1.934766 -1.428788
 O 1.882279 0.382067 -1.806385
 H -1.456086 -0.600079 1.860487
 H -2.106002 1.068289 0.823781
 H -0.865107 1.486659 1.663304
 H -0.811462 -1.815936 -1.213627
 H -1.912281 -1.978557 -0.051555
 H 0.594328 -1.964460 1.501090
 H 1.148041 -2.047734 0.018386
 H 0.412304 2.473124 0.296426
 H 1.326028 1.695290 1.274127
 H 1.410620 -0.501920 -1.762261

H 0.891750 -2.660351 -2.004818
 H 3.424305 0.280607 1.461527
 H 2.136758 -0.548937 1.068177
 H -0.844500 1.849785 -1.393496
 H -2.170675 -0.143697 -1.020858
 H -3.204259 0.968201 -1.482765
 H 2.315634 0.451214 -0.940344
 H 0.671112 1.650163 -1.686820

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oh2.9h2o, E= -763.345108
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 O -0.348582 0.153495 2.306601
 O -0.243027 -2.369983 1.097950
 O -2.662913 -2.360319 -0.442047
 O -2.221250 0.047372 -1.153396
 O -2.036270 1.710222 0.698320
 O -0.062485 3.153285 -0.635392
 O 1.629761 1.253487 0.626970
 O 1.681587 -2.058931 -0.826372
 O 3.833846 -0.233691 -0.035581
 H 0.467858 0.524550 1.922278
 H -1.044409 0.670331 1.851765
 H 0.119433 2.454953 -1.280758
 H -0.813109 2.785689 -0.120907
 H 1.034166 -2.249327 -0.102679
 H 2.455022 -1.658115 -0.395696
 H 1.129133 0.841004 -0.133597
 H 1.378071 2.186373 0.528131
 H -0.311130 -1.518878 1.584436
 H -1.091983 -2.458203 0.622307
 H -0.591186 0.131937 -1.428907
 H -2.701456 0.333193 -1.935908
 H -2.525515 -1.376133 -0.756330
 H 3.876737 -0.003061 -0.969513
 H 3.166157 0.390472 0.326305
 H -2.189427 1.022330 -0.086627
 H -2.902500 1.999232 0.996659
 H 0.812452 -0.618462 -1.484291

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oh2.9h2o, E= -763.343571
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 O 1.899824 1.447888 -1.136046
 O 2.488318 -1.200591 -0.864524
 O -1.835091 -0.607081 -1.833637
 O -0.083770 -2.567400 -0.981001
 O -0.782646 -1.835294 1.473131
 O -2.507728 -0.177778 0.834868
 O 1.563987 -0.739951 1.858316
 O 1.284010 1.921105 1.512315
 O -1.375692 2.338055 0.732411
 H -0.987628 0.889071 -1.924335
 H -2.247713 -0.478481 -0.953594
 H -1.202541 -1.346831 -1.675879
 H -0.484554 2.235177 1.129512
 H -0.925304 2.104288 -0.938748
 H 0.916301 1.583468 -1.473052
 H 1.784582 2.082736 0.698023
 H -0.352875 -2.395768 -0.030157
 H 0.822879 -2.229704 -1.038619
 H 1.395629 0.948396 1.696853

H 3.373881 -1.356819 -1.203238
 H 2.283184 -0.251953 -1.050485
 H -1.798319 -0.910379 1.176537
 H -1.017878 -2.524869 2.099278
 H -1.823823 1.475200 0.877679
 H -3.343575 -0.355905 1.272785
 H 2.018189 -1.044694 1.058185
 H 0.647329 -1.159775 1.792394

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oh2.9h2o, E= -763.343176
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 O 0.302529 0.094290 -1.036473
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 O -2.628958 2.227886 0.381394
 O -1.272332 -1.195407 1.853922
 O 0.549306 -2.353364 0.127804
 O 3.205402 -1.773909 0.398247
 O 2.997176 0.679215 -1.017576
 H -1.384657 0.320033 -1.732614
 H -2.588724 1.025325 -1.090914
 H -1.705445 1.948263 0.780388
 H 0.133388 0.535029 -0.161228
 H -0.151663 1.478317 2.128444
 H 2.761615 1.439915 -0.446090
 H 3.171972 -0.079906 -0.426648
 H 2.252459 -2.044348 0.410922
 H 3.617760 -2.381272 -0.223482
 H 0.018034 -2.110651 0.919777
 H 0.439428 -1.549298 -0.433274
 H -1.020204 -0.280943 1.599587
 H -1.957663 -1.456767 1.207742
 H -1.695535 -2.477769 -0.643435
 H -2.598395 -1.266558 -0.982895
 H 1.233713 0.320509 -1.255344
 O 1.770044 2.796199 0.328712
 H 1.449105 3.350193 -0.389457
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oh2.9h2o, E= -763.342945
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 O 2.081071 0.195920 -1.795836
 O -0.714391 0.779016 -2.237626
 O -2.901753 0.0733504 0.648799
 O -1.539605 2.304941 -0.140019
 O 0.435566 2.934748 1.415177
 O 2.412139 1.037313 0.824098
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 H -1.028796 -0.090535 -1.854272
 H -1.953151 -2.106357 -1.529749
 H -0.358759 2.705016 0.797472
 H 0.077012 -1.887374 -1.008691
 H 1.295243 -2.041583 -0.005280
 H 2.374161 0.877181 -0.141817
 H 1.762970 1.749203 1.010626
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 H 1.734083 -0.719352 -1.512344
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 H 2.258132 -1.612837 2.413815
 H 1.907900 -0.408030 1.467994
 H -1.214415 1.863797 -0.965316
 H 0.253801 0.711337 -2.229293
 H -2.111097 1.606647 0.262811
 H -2.492628 -0.465014 -0.081776
 H -2.519052 -0.374107 1.420247

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oh2.9h2o, E= -763.342856
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 H 0.980067 -2.004953 0.206782
 H 0.059609 0.856112 2.852300
 H 1.950534 2.230243 0.408487
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 H -1.965835 -1.205971 0.398580
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oh2.9h2o, E= -763.340703
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 O 0.034842 1.173485 0.366265
 O 2.878728 -1.161293 -1.194009
 O 2.181453 -1.289190 1.584250
 O -2.260955 -2.650019 -0.794223
 H -3.062871 0.547493 1.105355
 H 0.389171 3.232323 0.323097
 H 0.160806 2.207506 -0.786228
 H -1.304248 -1.123427 1.370976
 H -1.048670 -2.546169 0.921257
 H -2.740962 -1.911139 -0.387554
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H 0.098105 -1.174652 -0.311815	H 1.534786 2.709649 0.090522
H 2.291864 1.766334 0.128570	H 1.447944 1.734223 -1.075854
H 2.681145 0.550035 1.025421	H 0.448002 -0.387681 -1.333113
H 1.945920 -1.101893 -1.469323	H 0.179776 1.237052 -2.744390
H 3.082511 -0.262096 -0.862859	H -1.566556 1.923333 0.757406
H 1.239096 -1.522383 1.640659	H -0.514082 1.859661 -0.393098
H 2.457284 -1.527207 0.677845	H -3.076236 0.700349 -0.049449
H -1.756456 2.365633 0.065128	H -2.829235 0.218024 1.392100
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O -3.613684 -1.453302 0.165392	H 2.977612 1.025440 0.522397
O -3.154282 1.154381 -0.238979	31
O -0.902824 1.142274 1.108920	oh2.10h2o, E= -839.807519
O -0.811286 -1.394146 0.250228	O 2.262515 -1.223238 -1.489316
O -0.307979 1.858901 -1.067760	O 2.218220 1.366357 -1.309536
O 1.578495 0.589924 2.210396	O 2.277731 1.402801 1.402997
O 1.773027 -1.876797 1.096929	O -0.348922 2.018450 1.258205
O 2.811864 -0.909100 -1.121975	O -1.867393 0.020986 1.923388
O 2.379120 1.770880 -0.204420	O -0.451628 -2.078753 1.440116
O 0.192021 -0.709856 -2.221602	O -0.423104 2.079055 -1.194048
H -3.949068 -1.418127 1.066614	O -0.371915 -2.180064 -1.355863
H -3.530699 -0.495977 -0.098678	O -2.004270 -0.029977 -1.909524
H -2.731837 1.432508 -1.061717	O -3.937707 -0.038187 -0.128578
H -2.365565 1.198973 0.388093	O 2.287815 -1.442527 1.351118
H -0.775395 -0.443182 0.536752	H 2.245142 -0.208472 -1.481426
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H 1.145112 -0.795638 -2.046384	H 2.406683 -1.480760 0.384999
H 2.469811 -1.337720 -0.278041	H 1.350135 -1.683222 1.483003
H 3.594694 -1.399819 -1.384824	H -1.427088 0.742352 -1.697195
H 1.778106 -1.048484 1.643848	H -3.217731 -0.044794 -0.855715
H 0.827271 -1.970851 0.862491	H 1.311789 1.635433 1.457998
H 1.460551 1.912619 -0.527632	H -0.555584 2.832090 1.726689
H 2.657847 0.940148 -0.626948	H -1.433684 -0.824229 -1.783518
H 0.623976 0.723994 2.001884	H 2.380801 1.473379 -0.335147
H 2.006657 1.090504 1.482509	H 1.285528 1.668634 -1.410827
H -0.563370 2.015823 0.880203	H -0.701460 2.937922 -1.522733
H -0.214805 0.961358 -1.462203	H -0.426494 2.117963 -0.093372
H -1.763109 -1.619120 0.248413	H -0.448864 -2.250415 -0.383652
31	H 0.549497 -1.892029 -1.505545
oh2.10h2o, E= -839.809614	H -1.011448 -1.250982 1.642906
O -1.798360 -2.326206 -0.745013	H -0.769518 -2.771364 2.025293
O 0.594025 -1.243495 -0.766971	H 2.319928 0.436483 1.547749
O 0.055406 0.978854 -1.827368	H -2.626821 0.057072 1.315110
O -2.509119 0.154134 -1.712364	H -1.290986 0.828989 1.703686
O -1.919032 -1.324277 1.996262	31
O 2.107785 2.221362 -0.514598	oh2.10h2o, E= -839.805688
O -3.121563 1.000406 0.882859	O 3.968600 -0.363636 -0.644166
O -0.630434 2.141093 0.544229	O 2.238005 0.236993 1.599060
O 0.557124 -0.032177 1.690039	O 0.843201 -1.731534 0.103652
O 3.199087 -1.983233 -0.570162	O 1.162460 -0.039909 -1.738643
H 2.258123 -1.758461 -0.780688	O -0.313099 -1.005454 2.487605
H 3.141065 -2.778674 -0.032012	O -2.400015 0.520671 1.541322
H -0.833223 -2.013456 -0.819234	O -1.355378 2.552905 0.321607
H 0.580178 -0.883193 0.153829	O -1.422658 1.078371 -2.071559
H -2.476654 -0.811041 -1.786798	O -3.045336 -0.792704 -0.774101
H -1.563298 0.467426 -1.795865	O 1.395785 2.282925 -0.087764
H -1.931794 -1.854637 1.182180	O -1.244857 -3.015991 -0.723044
H -1.006875 -0.982489 2.060488	H 3.704578 -0.154025 0.268056
H 1.535815 0.080826 1.720342	H -2.540675 -0.178861 -1.350653
H 0.184436 0.826392 1.365179	H -2.739550 -0.014635 0.782604

H -1.698670	-0.032135	1.959097	O 0.972970	3.738299	-0.563849
H -2.525962	-1.619788	-0.776693	O -3.345564	0.991784	0.711509
H -0.402534	-2.527226	-0.378324	O -2.832605	0.009363	-1.890637
H -0.525188	0.699515	-1.991518	H 3.274433	0.025563	-1.556912
H -1.466615	1.742314	-1.358793	H 3.073955	-0.784378	-0.232379
H 0.421249	-0.420480	2.724185	H 1.577965	1.289219	1.113308
H 0.018657	-1.411806	1.650904	H 2.881817	1.318011	0.307862
H 1.395152	1.656427	-0.830568	H -1.997337	-1.699569	1.257914
H 0.452040	2.456435	0.097283	H -2.596991	-0.354926	1.684985
H 1.762875	-0.442381	1.075463	H -0.413765	1.081671	-0.093334
H 1.993118	1.075581	1.152545	H -0.386083	2.514397	-0.703972
H 3.170664	-0.132237	-1.141530	H -0.618722	-1.214958	-0.301322
H 1.027458	-0.777429	-1.006450	H -0.567673	-2.637297	-0.875697
H -1.814598	3.352304	0.591173	H 1.070379	-0.849413	0.888878
H -1.752993	1.786409	0.856358	H 2.616931	-2.220439	1.242001
H 1.583170	-2.348018	0.137614	H 1.498769	-2.963691	-0.300146
H 1.324165	-0.491056	-2.572512	H -2.558694	1.517147	0.472635
31			H -3.525550	0.551935	-0.142260
oh2.10h2o,	E=	-839.805321	H -2.155520	0.693586	-1.740269
O 0.692691	-2.579071	0.461155	H -2.366069	-0.813045	-1.648935
O -1.496287	-0.835785	-2.056245	H 1.556834	3.098790	-0.068303
O -0.586954	0.387220	1.737553	H 0.757233	4.421658	0.077681
O -2.241538	2.447852	0.705787	H -0.338967	-0.414653	1.615093
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oh2.10h2o,	E=	-839.803492	oh2.10h2o,	E=	-839.803492
O -2.038925	-1.544652	-1.038119	O -2.038925	-1.544652	-1.038119
O -2.400750	-0.944532	1.309293	O -2.400750	-0.944532	1.309293
O 0.366681	-2.358891	-0.901842	O 0.366681	-2.358891	-0.901842
O -2.314881	1.685091	0.985907	O -2.314881	1.685091	0.985907
O 2.166959	-0.398852	-1.774072	O 2.166959	-0.398852	-1.774072
O 0.653330	1.833967	-1.814818	O 0.653330	1.833967	-1.814818
O -2.045578	1.063055	-1.836077	O -2.045578	1.063055	-1.836077
O 3.931379	-0.136388	0.165503	O 3.931379	-0.136388	0.165503
O 1.867998	0.444092	2.136683	O 1.867998	0.444092	2.136683
O 0.448055	2.455790	0.883005	O 0.448055	2.455790	0.883005
O 0.229577	-1.788094	1.848982	O 0.229577	-1.788094	1.848982
H -0.614609	-2.073768	-1.033918	H -0.614609	-2.073768	-1.033918
H -2.704493	-2.050105	-1.511730	H -2.704493	-2.050105	-1.511730
H 3.274447	-0.229219	-0.611593	H 3.274447	-0.229219	-0.611593
H 1.630475	0.435225	-1.850274	H 1.630475	0.435225	-1.850274
H -2.272851	1.473259	-0.987076	H -2.272851	1.473259	-0.987076
H -2.036769	0.094274	-1.632232	H -2.036769	0.094274	-1.632232
H -2.392488	0.713549	1.194632	H -2.392488	0.713549	1.194632
H -2.849524	2.153202	1.632213	H -2.849524	2.153202	1.632213
H 0.461541	-3.231641	-1.291763	H 0.461541	-3.231641	-1.291763
H 1.526481	-1.090621	-1.513076	H 1.526481	-1.090621	-1.513076
H -0.281383	1.573841	-1.960909	H -0.281383	1.573841	-1.960909
H 0.408819	-2.089139	0.937023	H 0.408819	-2.089139	0.937023
H -0.697074	-1.479898	1.804903	H -0.697074	-1.479898	1.804903
H -3.121931	-1.428516	1.719252	H -3.121931	-1.428516	1.719252
H -2.318892	-1.265928	0.264659	H -2.318892	-1.265928	0.264659
H -0.484303	2.200392	0.990051	H -0.484303	2.200392	0.990051
H 0.667050	2.140047	-0.879385	H 0.667050	2.140047	-0.879385
H 0.966046	1.772399	1.368957	H 0.966046	1.772399	1.368957
H 1.303265	-0.359282	2.091222	H 1.303265	-0.359282	2.091222
H 2.625439	0.257239	1.553494	H 2.625439	0.257239	1.553494
31			31		
oh2.10h2o,	E=	-839.803396	oh2.10h2o,	E=	-839.803396
O 0.549409	-1.617981	1.960812	O 0.549409	-1.617981	1.960812
O -1.587909	-0.137736	2.072771	O -1.587909	-0.137736	2.072771

O -1.389046 2.288304 1.006264
 O 2.858540 -1.008016 0.405088
 O 3.252479 1.751612 0.456159
 O 0.959725 2.497202 -0.241363
 O -0.016965 0.568592 -1.610196
 O 1.678503 -1.640040 -1.999726
 O -0.423697 -2.483922 -0.487536
 O -2.778961 -1.329148 -0.221748
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 H 0.679525 -2.041072 2.813387
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 H 0.301733 -2.299180 -1.137557
 H 2.284289 2.107992 0.198556
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 H -1.778782 1.166553 -1.694153
 H 3.057838 -0.044672 0.446320
 H -2.176888 -0.540261 1.409985
 H -1.478334 0.810191 1.768137
 H -0.473322 2.424511 0.624503
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 H 2.239322 -1.446710 -1.210621
 H 2.109244 -1.141217 1.011891
 H 1.257764 -0.779749 -2.188065
 H -3.449778 -2.011355 -0.311061
 H -1.905349 -1.770216 -0.429367
 H 0.417232 1.367243 -1.127122
 H -0.209855 -0.061912 -0.904511

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oh2.10h2o, E= -839.802248
 O 0.201459 -0.629932 -0.383538
 O -2.119520 -1.398656 -1.432835
 O -1.770110 -2.715462 1.077801
 O 1.256113 -2.851171 -0.017622
 O -2.897701 1.059009 -0.864106
 O -1.497941 0.140962 1.430981
 O 0.100896 2.392795 1.882890
 O -0.532276 2.745688 -0.842963
 O 3.472989 -1.016257 -0.706929
 O 1.911130 1.554413 -1.392321
 O 2.128004 0.465514 1.314314
 H -0.852141 -2.932725 0.852703
 H -1.180368 -1.147489 -1.200566
 H -2.322455 -2.011346 -0.702372
 H 2.121143 1.508777 -0.445039
 H 1.054927 2.039323 -1.403373
 H -0.827631 -0.078165 0.708465
 H 1.369666 -0.003865 0.898238
 H 2.889807 -0.000797 0.927556
 H 0.808164 -1.906411 -0.227123
 H 2.866336 -1.770023 -0.589649
 H -1.320331 2.180999 -0.934946
 H -0.339905 2.754158 0.119361
 H 0.975040 1.969934 1.863310
 H -2.712997 0.118878 -1.159579
 H -3.710553 1.337835 -1.293333
 H 0.639317 -0.004330 -0.978452
 H 2.992099 -0.393530 -1.272387
 H -0.513830 1.632853 1.955742
 H -2.233145 0.533414 0.934177

H -1.727485 -1.802718 1.421900
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 oh2.10h2o, E= -839.801865
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 O 1.976144 -2.178518 1.461758
 O 0.748569 -2.929511 -1.008382
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 H 2.990122 -1.066697 0.281335
 H 1.358355 -1.447916 1.645306
 H 1.534846 -2.657074 0.734955
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 H 0.204545 -0.111532 0.254719
 H -3.038714 -0.835872 -0.770400
 H -4.536630 -1.196428 -0.502271
 H -3.023156 -0.589670 1.280266
 H -2.696764 0.885856 1.561893
 H -1.089245 -0.041685 -1.575908
 H -1.964233 1.053354 -0.914703
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 H 0.764738 -0.334381 -2.503685

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oh2.10h2o, E= -839.801419
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 O -1.066835 -1.301829 -2.185161
 O 0.547028 1.001682 -1.295484
 O -3.096876 -0.714655 -0.387211
 O -1.313199 3.049687 -1.000222
 O -2.196964 1.410294 0.692074
 O -2.305172 -1.804373 2.189940
 O 0.754822 -2.236858 -0.308983
 O 2.088191 1.699858 1.372037
 O 4.043718 -0.211563 0.909435
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 H -1.840606 -1.125107 -1.606727
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 H -2.693380 -1.617174 1.319332
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 H -0.043810 1.787360 -1.340009
 H -0.939925 0.564869 1.168324
 H -2.716068 1.714933 1.441681
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H 3.819162 -0.985594 1.435941
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 H -3.986999 -0.581649 -0.723887
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oh2.10h2o, E= -839.799932
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 O -1.478453 3.400739 -0.422006
 O 0.722605 1.797252 -0.653791
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 O -0.305662 -2.041435 -0.459959
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 O 2.382027 -0.262104 1.974248
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 H 2.818746 0.367270 1.367398
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 H 2.411914 -1.690256 0.893108
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 H -1.962397 2.658949 0.092231
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 H 0.549688 -2.405084 -0.133633
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 H -3.144303 1.584516 1.567373

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oh2.10h2o, E= -839.799669
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 O 0.328978 -0.406615 -1.442362
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 O -2.214088 -2.035152 1.343423
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 O -0.674033 1.865923 0.860152
 O 1.630205 3.242003 0.894843
 H 0.297255 -0.692055 0.028309
 H 1.126944 -0.861604 1.376861
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 H 2.964702 -0.178322 0.327771
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 H 0.716539 2.816841 0.957777
 H 2.397056 -2.414331 -0.102819
 H 0.952307 -2.792470 -0.363138
 H -0.437290 0.966940 -1.903706
 H -1.903276 1.410112 -2.051847
 H -0.337914 0.954824 1.035962
 H -0.857659 1.890576 -0.113767
 H 0.722499 -1.103181 -1.977274

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oh2.10h2o, E= -839.799635
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 O 1.599151 2.389387 -0.962860
 O -0.455458 2.774361 0.622355
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 O 3.058428 0.790901 0.991919
 H -0.510667 -0.871358 -1.838747
 H -0.306020 -2.728610 -0.585149
 H -0.317160 -2.564926 0.950561
 H -1.802830 2.337179 0.066369
 H -0.490340 3.520871 1.225052
 H 3.146131 -0.083561 0.581146
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 H 1.592667 -0.577912 -1.370359
 H 1.090375 0.921452 -1.541455
 H 0.829750 2.674571 -0.375512
 H 2.274058 2.061196 -0.340727
 H -2.057650 -1.348104 1.383063
 H -2.802989 -1.036933 -0.826378
 H -0.761175 -0.813027 1.998461
 H 3.100060 -2.461837 -0.681751
 H 1.696562 -2.242110 -0.015082
 H -0.023714 1.439175 1.197398
 H 0.340805 0.128190 0.443223
 H -2.538630 2.135650 -1.312459

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oh2.10h2o, E= -839.799503
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 O -0.269995 0.014724 -2.424281
 O 2.214766 -0.208801 -1.749915
 O 1.855362 -2.257567 -0.196016
 O 2.805168 1.362134 0.202641
 O 0.382938 2.317423 0.792108
 O -1.507638 2.218204 -0.998605
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 O 1.944169 -0.613252 2.280671
 H -2.328889 -2.039821 -0.212091

H -0.642369	-1.077941	-1.270340	O -3.173380	-1.367577	0.664166
H 0.156211	-2.117056	-0.386469	O 3.628034	1.497836	-0.069325
H 2.033170	-1.856905	0.668594	O 2.326455	-2.054027	-0.265785
H 2.079862	-1.515617	-0.859695	O -2.316256	0.941785	2.086026
H -0.676556	-0.711094	0.912453	O -2.323152	2.335578	-0.331513
H -1.578481	0.244856	1.716379	O -0.458422	-2.033182	0.585543
H 0.989645	-0.385119	2.229771	H 2.836700	-1.138848	1.218558
H 2.082764	-0.963099	3.164917	H 3.375137	0.288072	1.339027
H 2.845108	0.740603	0.943100	H -2.352664	1.965950	0.579938
H 2.630313	0.773022	-0.617223	H -2.763374	0.867447	-1.254177
H 0.735366	0.007836	-2.246158	H -2.040501	-0.363037	-1.908767
H 2.863552	-0.278414	-2.454910	H -1.376115	2.441523	-0.524549
H -0.619203	0.860400	-2.101046	H 1.078428	1.189211	-1.280328
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O 1.855321	-1.116836	-1.718958	H -4.016184	-1.826603	0.709011
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O 2.649647	2.778340	-1.188642	O -1.514643	1.690508	-0.331636
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H -3.070921	0.314358	0.243242	H -0.816491	2.315283	-0.041514
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O 0.057036	-0.609973	-1.785130	H 2.374420	1.805596	-1.106719
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O -1.445835 -2.231202 1.216620	H 3.206279 -1.188807 -0.299131
O -1.298916 -1.990950 -1.545758	H 3.589075 -0.032713 0.585910
O -2.843898 0.067124 -2.252549	H -0.360194 -0.051466 -2.714085
O 1.324906 -2.750139 1.003682	34
O 2.431049 -0.200236 1.552276	oh2.11h2o, E= -916.261426
H 1.183019 0.856509 2.153184	O -1.851551 2.341606 -0.604271
H -0.116071 3.972189 0.116342	O -0.398747 0.051229 -1.370891
H 0.332422 2.057841 1.644758	O 1.601990 1.403060 -0.164327
H 3.695867 0.207443 -1.323632	O 1.580365 -0.261426 2.113323
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H -0.331360 -1.863718 -1.654718	O 0.623527 -2.279180 -0.961147
H -1.422883 -2.139186 -0.586035	O 3.168818 -1.883739 0.349006
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O -1.163623 3.732132 0.056520	oh.6h2o, E= -534.645268
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 H -1.904016 -1.445282 -0.199031
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 H 1.916283 1.605884 -0.167385
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 H 1.577829 -0.640401 -0.687713
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oh.6h2o, E= -534.642390
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 O -2.903967 -0.990088 -0.175332
 O -0.199736 -1.554159 -0.141735
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 H 1.586047 1.178876 0.210854
 H 1.054358 1.471420 -1.192050
 H 2.216869 -0.866156 0.608698
 H 2.731054 -0.411259 -0.709176
 H -0.609406 0.953615 1.347437
 H -2.101092 0.594114 1.066155
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 H 0.617828 -1.923209 -0.503326
 H -2.746979 -0.342454 -0.876316
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 H -0.563749 -0.035698 -1.245142
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 O 1.500532 -1.173988 0.995951
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 H -0.561454 -1.457719 -1.184821
 H -1.582249 -1.041069 0.654704
 H -2.579452 -0.794838 -0.449757
 H -1.908590 1.754566 -0.807670
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 H 1.208891 -1.466038 0.110230
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 H 2.620432 0.018030 0.466059
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 H 0.043020 1.133142 0.261671

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 O 0.688537 -0.904176 1.952873

O -0.398052 1.703435 1.351705
 O 1.025263 1.756923 -0.854803
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 H -1.924752 0.984649 0.280355
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 O 1.013548 1.804640 0.371140
 O -1.128685 -1.458190 -1.322390
 O -2.555892 0.015418 0.693357
 O -1.129364 1.431471 -1.371004
 H 0.279317 0.691765 1.621812
 H -1.779982 -0.043807 1.294288
 H -2.286718 0.703574 0.056203
 H -0.987293 0.490143 -1.586840
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oh.6h2o, E= -534.641114
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 H 0.153352 0.544724 1.795160
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 H -2.286191 0.774423 -0.063832
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 H 1.704037 2.575703 0.807331
 H 1.705430 1.137872 0.152069
 H 1.886661 -0.878071 -0.239495
 H 2.112911 0.007275 -1.565469
 H -1.702683 -1.138327 -0.824651
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H 0.176167 -0.957942 1.461429
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 O 0.468469 1.869076 -1.021762
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 oh.6h2o, E= -534.638951
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 O 2.254535 -0.262660 -1.533591
 O 0.375671 -2.143528 -0.626910
 O -4.144580 0.441547 -0.136649
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 H 0.260830 2.296231 -1.330033
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 oh.6h2o, E= -534.638335
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23
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23
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H -2.162240 -1.505091 0.792902	23
H -0.848350 1.269113 1.458363	oh.7h2o, E= -611.106661
H -0.041985 0.009335 1.871075	O -0.127962 -1.366119 -1.627815
H 0.083436 -1.704401 0.356796	H -0.364234 -1.884372 -2.400638
H 1.250903 -1.680456 1.300359	O -1.899664 -1.263374 0.065378
H 1.748408 -1.145370 -0.770069	H -0.961993 -1.397928 -0.918458
H 2.545940 -0.060854 -0.050321	H -2.573205 -1.946848 0.099911
H 1.301464 1.525917 0.981395	O 0.138803 1.363222 -1.612819
H 1.348059 1.668120 -0.541599	H 0.043483 0.394362 -1.760324
H -0.065592 -1.951061 -1.987842	H 0.034647 1.449417 -0.648854
23	O 2.089290 -1.538295 0.047487
oh.7h2o, E= -611.107008	H 1.386551 -1.565622 -0.635250
O 0.715186 -0.471717 -1.552785	H 2.384766 -0.607960 0.056849
H 0.937156 -0.688518 -2.462477	O 0.007578 -1.151924 1.951695
O 2.679175 0.829546 -0.254491	H -0.757927 -1.304375 1.333966
H 1.987104 0.440495 -0.857567	H 0.790455 -1.424990 1.433317
H 2.891861 0.069642 0.303867	O -0.028438 1.509234 1.344429
O 1.727448 -1.914409 0.617833	H 0.015698 0.577111 1.679807
H 1.451617 -1.503834 -0.232854	H -0.969549 1.616684 1.093485
H 1.169514 -1.465063 1.274372	O 2.526491 1.312926 0.012726
O -1.210799 -1.791472 -0.552259	H 2.076462 1.417433 -0.841931
H -0.461833 -1.286296 -1.053731	H 1.805120 1.525389 0.633296
H -0.770061 -2.551706 -0.158082	O -2.508611 1.298609 0.023183
O -0.977573 1.646500 -1.249585	H -2.386121 0.299604 0.061120
H -0.372952 0.890718 -1.469891	H -2.104049 1.537853 -0.820399
H -1.782358 1.234375 -0.890533	23
O 0.526034 2.085357 1.037406	oh.7h2o, E= -611.105635
H -0.041681 2.127553 0.234995	O 0.340913 -0.387719 -1.569448
H 1.390575 1.792109 0.680952	O 2.266717 1.305269 -0.820316
O -0.464331 -0.344058 1.873251	O 2.145532 -1.718975 -0.216277
H -0.103604 0.549184 1.650871	O -1.399122 1.474330 -0.676548
H -0.743470 -0.728493 1.025207	O 0.517898 2.066800 1.268405
O -3.038375 0.145364 0.205189	O 0.658920 -0.644159 2.006949
H -2.591576 -0.670006 -0.100257	O -3.408446 -0.099053 0.047042
H -2.614405 0.308950 1.058657	O -1.121948 -1.808509 0.208486
23	H -3.834062 -0.253864 -0.801499
oh.7h2o, E= -611.106674	H -2.694445 0.573301 -0.159705
O 2.083700 1.637560 0.013439	H -0.656462 -1.330908 -0.528030
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O -0.061189 1.133251 -1.724481	H 1.707964 -2.535125 0.047701
O 2.522411 -1.125802 -0.214145	H -0.779694 0.817138 -1.095024
O -0.135894 -1.685778 1.440925	H -0.863652 1.834616 0.063370
O -2.529636 -1.176097 -0.172404	H 1.211528 1.983405 0.582845
O 0.069475 -1.433587 -1.191538	H 0.509730 1.173493 1.674294
H 2.422894 0.724543 -0.095228	H -0.100392 -1.053251 1.534285
H 1.463110 1.550879 0.769164	H 1.393860 -0.873677 1.411039
H 0.081493 0.097105 1.832518	H 1.524162 0.768930 -1.221192
H -0.675020 1.368406 1.404441	H 2.822334 0.620885 -0.429177
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H -1.235038 1.488278 -0.718297	23
H 0.751334 1.432901 -1.261220	oh.7h2o, E= -611.104970
H -0.014908 0.128953 -1.658972	O -0.018090 0.008377 -1.559780
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H -1.682655 -1.308092 -0.659658	

O 3.535281 -0.027744 0.053069
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 H 0.120152 -1.173115 1.495220
 H 2.878428 0.690042 0.035550
 H 0.800966 -1.081537 -0.669251
 H 0.233952 -0.068656 -2.484131
 H 2.978618 -0.820647 0.084180
 H 0.658680 -2.535383 -0.153708

23

oh.7h2o, E= -611.104777

O 0.613606 0.997314 1.345827
 H 0.790457 1.464488 2.166944
 O 2.072650 -1.229931 1.135845
 H 1.629887 -0.343247 1.268260
 H 1.371535 -1.834564 1.412009
 O 1.510776 1.875088 -0.900035
 H 1.243834 1.580584 0.042348
 H 2.413727 2.197190 -0.832152
 O -1.321377 2.270705 -0.024307
 H -0.702603 1.813434 0.609569
 H -0.725689 2.476920 -0.755628
 O -0.953098 -1.307949 1.520054
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 H -0.840225 -1.671737 0.617288
 O -2.847138 -0.032638 -0.365300
 H -2.536382 -0.453399 0.454228
 H -2.408815 0.845224 -0.342194
 O -0.906347 -1.948427 -1.232685
 H -1.584972 -1.248835 -1.261076
 H -0.058973 -1.536694 -1.509291
 O 1.630355 -0.853695 -1.619230
 H 1.565622 0.118909 -1.547591
 H 1.908951 -1.118095 -0.716918

23

oh.7h2o, E= -611.104614

O -0.437006 1.027292 -1.240866
 O -1.816350 -0.907527 1.670810
 O 1.456498 1.857700 0.473589
 O 3.454003 -0.292572 -0.188787
 O 0.987641 -1.109024 -1.176948
 O 1.014994 -0.639692 1.609865
 O -1.991765 -1.336809 -1.158068
 O -2.652728 1.371669 0.205236
 H -2.091520 -0.006495 1.410096
 H -0.851996 -0.841946 1.817489
 H -1.536120 -0.485395 -1.329397
 H -1.972741 -1.397117 -0.182166
 H -1.793650 1.381649 -0.308875
 H -3.174332 0.726832 -0.288013

H 0.726750 1.669526 -0.181999
 H 2.248554 1.465641 0.075068
 H 0.487126 -0.222392 -1.282840
 H 0.299906 -1.763336 -1.356833
 H 3.147764 -0.486315 0.707802
 H 2.749738 -0.695474 -0.732249
 H 0.973607 -0.980273 0.692722
 H 1.102351 0.327121 1.454627
 H -0.437735 1.539684 -2.054076

23

oh.7h2o, E= -611.104284

O 0.000007 -0.000124 -1.786355
 O 0.524740 1.964624 -0.208671
 O -0.524879 -1.964781 -0.208451
 O 0.000114 0.000061 1.757590
 O -2.729121 -0.723078 1.165969
 O 2.729272 0.723413 1.165702
 O -2.277317 1.335813 -0.877667
 O 2.277209 -1.335931 -0.877522
 H -1.563978 0.818150 -1.317332
 H -2.622667 0.721193 -0.207301
 H -0.363659 2.349760 -0.216354
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 H 1.563813 -0.818370 -1.317245
 H 2.622617 -0.721167 -0.207322
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 H -2.029635 -0.306212 1.696724
 H 2.220426 1.392813 0.676975
 H 2.029873 0.306545 1.696572
 H -0.000107 -0.000035 -2.746186
 H -2.220400 -1.392664 0.677366

23

oh.7h2o, E= -611.104046

O 0.019525 -1.170665 2.074025
 O 2.302636 -0.204674 0.821391
 O 0.870615 2.276672 0.165712
 O 0.112009 0.998219 -1.953841
 O 1.278078 -1.167861 -1.397077
 O -0.863205 -2.250712 -0.331639
 O -2.389245 0.235840 -0.712040
 O -1.288901 1.131330 1.528645
 H 0.911655 -0.887469 1.763659
 H -3.335329 0.400669 -0.692011
 H -2.025642 0.591815 0.152696
 H 0.588965 1.819904 -0.701767
 H 1.133252 3.169888 -0.069977
 H -1.510661 -1.564169 -0.554770
 H -0.327585 -1.687368 1.309380
 H -0.552973 1.677412 1.188719
 H -0.844788 0.301453 1.854845
 H 2.028653 0.719065 0.712457
 H 2.025926 -0.630295 -0.050453
 H 1.796032 -1.626912 -2.062174
 H -0.021269 -1.942563 -0.795514
 H 0.621318 0.093517 -1.825864
 H -0.819649 0.779855 -1.790633

23
oh.7h2o, E= -611.103703
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O -1.735955 1.448528 -1.213500
O -0.483550 1.725004 1.380546
O -1.055752 -0.780997 1.904932
O 0.265505 -1.791822 -0.104471
O 0.629718 0.186675 -1.931365
O 2.055456 1.595777 0.121804
O 2.763080 -1.102812 0.261153
H -1.555721 -1.484305 -0.539870
H -2.429308 -0.258663 -0.811158
H -0.931905 1.061222 -1.630819
H -1.415079 1.726274 -0.338921
H -0.635034 2.258532 2.165059
H -0.689126 0.770907 1.640473
H -1.891225 -0.884318 1.413728
H -0.432874 -1.252426 1.260200
H 1.195675 0.759333 -1.378243
H 0.478550 -0.616044 -1.368257
H 1.223753 1.705900 0.619509
H 2.387905 0.707263 0.368743
H 1.799620 -1.417023 0.190080
H 3.051971 -1.087299 -0.657552
H 0.261376 -2.742698 -0.246546

23
oh.7h2o, E= -611.102161
O -0.921844 -1.081324 -1.226490
O -0.114981 -2.159279 0.990770
O 0.149859 0.489033 2.034477
O 1.711014 -1.474159 -1.278139
O -1.482919 1.498980 -1.544706
O -2.532511 -0.075027 0.844853
O 2.754666 0.632536 0.157860
O 0.565618 2.419377 0.066428
H -2.067366 -0.491625 0.085571
H -1.807011 0.233282 1.413413
H -0.489376 -1.833241 0.107487
H -0.889518 -2.250796 1.555608
H 0.741216 -1.254329 -1.409854
H 1.672429 -2.139486 -0.580214
H -1.218918 0.534112 -1.567700
H -2.146681 1.496152 -0.841105
H -0.095851 2.171295 -0.618091
H 1.403094 1.986109 -0.179898
H 2.326153 0.478674 1.010563
H 2.439287 -0.107932 -0.412545
H 0.240846 1.193969 1.353765
H 0.232028 -0.373639 1.585801
H -1.371543 -1.643640 -1.863222

23
oh.7h2o, E= -611.101899
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O -0.412356 -1.765805 0.376496
O -1.105181 0.996972 -1.701304
O -2.829907 -0.945370 -0.355788
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O -0.258381 2.339953 0.580691

H 2.225636 -1.243052 -0.215380
H 1.904498 -1.980038 1.062020
H 1.899696 0.779155 -0.673841
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H -0.280554 0.434259 -1.665029
H -1.809447 0.416390 -1.370663
H -3.373901 -1.603574 -0.796247
H -1.967649 -1.399651 -0.131453
H 0.152701 -1.357976 -0.352704
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H -0.627669 2.029146 -0.276857
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23
oh.7h2o, E= -611.101312
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O -2.567783 -0.331986 -0.918168
O 0.177309 0.181336 1.560051
O 0.829908 -1.590003 -1.176310
O -1.988231 2.017606 0.885673
O 2.771177 -0.825148 0.675488
O -1.212900 -2.151427 0.756129
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H 0.176197 -2.028518 -0.599531
H -1.840115 -1.627476 0.219177
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H 0.222379 0.456600 0.615782
H -0.489149 0.797671 1.900120
H 2.198209 -1.217025 -0.021771
H 2.128944 -0.517100 1.331761
H -1.684630 0.164653 -1.056382
H -2.773823 -0.737320 -1.765043
H 1.600417 1.585353 -0.680434
H 2.868585 0.911377 -0.201630
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26
oh.8h2o, E= -687.568371
O -1.027785 -1.595726 -1.444712
O 1.277495 -0.479180 -1.463815
O -0.813632 -2.070089 1.318778
O -0.137222 1.895223 -1.348563
O 1.941756 -1.842877 0.773696
O 2.762081 0.992238 0.191734
O 0.317452 2.086148 1.356974
O -1.941232 0.458814 1.793982
O -2.609927 0.673438 -0.898361
H -2.241361 -0.179662 -1.191173
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H 0.368042 1.061034 -1.495617
H -1.073778 1.601169 -1.300662
H 2.652588 1.917147 -0.051381
H 2.227036 0.485775 -0.486462
H -0.095601 -1.160655 -1.503371
H 1.768915 -0.635290 -2.275343
H 0.121495 2.148764 0.390469

H 1.112818 1.532503 1.365422	H -1.395226 1.267859 1.741357
H -1.164501 1.055284 1.783285	H 0.397839 1.593022 -0.821653
H -1.560231 -0.444601 1.764981	H 1.625265 2.172873 -0.114667
H 1.725436 -1.477590 -0.124871	H 0.214095 0.353942 -2.705115
H -1.015115 -2.026873 0.364084	
H 0.164387 -2.036580 1.328939	
H -1.037902 -2.321372 -2.073792	
H 2.406154 -1.104650 1.186114	
26	
oh.8h2o, E= -687.567214	26
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O 2.044594 1.446012 0.738352	O 1.610515 2.288916 0.264713
O 0.697762 -0.767668 -1.462397	O 1.513071 0.531401 -1.870043
O 3.520977 -0.405537 -0.715541	O -1.157680 0.055505 -1.597369
O -1.905990 1.473853 1.260942	O -0.347584 -2.242469 -0.527971
O -1.416420 -1.217923 1.864971	O -1.127647 -0.883550 1.718342
O -1.843671 -1.920300 -0.814948	O 1.557413 0.043898 1.850363
O -2.665947 0.710611 -1.389549	O 2.387156 -1.546040 -0.091596
O 1.364591 -1.221948 1.226882	O -3.296780 -0.094327 0.064292
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H -1.140482 1.660232 0.663529	H -1.053062 1.202137 0.984506
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H 1.602562 -0.277902 1.321057	H -0.654830 -1.453625 -1.059891
H 1.187472 1.605555 0.147909	H 0.621380 -2.187139 -0.513519
H 2.104631 2.172423 1.363525	H 1.930988 -0.238505 -1.451806
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H -1.760525 -1.778089 0.154457	H 0.640081 2.420745 0.298460
H -0.951665 -1.747491 -1.160010	H -0.812220 -1.490377 1.002738
H 3.197024 0.410691 -0.284357	H -2.020895 -0.654711 1.393872
H 0.403007 0.177719 -1.279827	H 2.120303 -0.983035 0.694519
H 1.653306 -0.708989 -1.620467	H 3.196505 -2.000996 0.153451
H 0.039273 2.384164 -1.303056	H -2.583539 -0.175493 -0.629859
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O 0.188385 0.299525 -1.746716	
O 2.881846 0.566689 -0.907716	
O 2.623847 -1.550441 1.058516	
O 0.248945 0.072373 1.736083	
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H -2.662620 -2.023441 0.920354	
H -2.609572 -1.224226 -0.403259	
H -1.456085 0.354868 -1.328639	
H -2.364571 0.988774 -0.230893	
H 2.011352 0.374598 -1.319952	
H 2.992083 -0.149095 -0.255910	
H 2.144770 -0.971598 1.670938	
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H 0.112639 -0.647402 1.080916	
H 0.530585 0.825799 1.176775	
H -1.057117 2.438504 0.862656	

26

oh.8h2o, E= -687.565780
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 O -0.303541 -1.916753 -0.815386
 O -1.946400 0.193110 1.693912
 O 1.693813 1.345133 1.515052
 O -2.946439 -1.029466 -0.741696
 O -2.022316 1.707686 -0.653945
 O 0.733129 2.172263 -1.009916
 O 1.627228 -0.218835 -2.075095
 O 2.929703 -0.981123 0.293416
 H 2.071230 -1.125141 0.737266
 H 2.657830 -0.721122 -0.612859
 H 2.485795 0.909280 1.159890
 H 1.106206 0.561831 1.641490
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 H -1.965495 1.376714 0.264548
 H -1.040082 -0.289317 1.655850
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 H 1.038846 2.010498 -0.092694
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 H 1.344675 0.686426 -1.806887
 H 0.882544 -0.785508 -1.802897
 H -2.906697 -0.748593 0.186251
 H -0.042716 -1.615773 0.133524
 H 0.402924 -1.653665 2.213474
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 H 0.033194 -2.811578 -0.914844

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 O -2.417801 -0.599111 -1.676214
 O 2.762710 -1.260332 0.496680
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 H -1.662805 -0.754412 -2.255751
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 H -0.214270 0.351624 2.245121
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 H -2.298297 1.141317 -1.082072
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 H 0.644556 0.340930 -1.123299
 H 2.100102 -0.940950 1.134318
 H 3.178175 -0.442786 0.165783
 O 3.446358 1.374442 -0.426048
 H 2.471444 1.419034 -0.598912
 H 3.577739 1.926678 0.350810

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 O 2.049560 -1.631850 -0.570617
 O -1.059391 2.517991 -0.560045
 O 0.675448 1.231618 1.445900
 O 0.864092 0.678109 -1.258779
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 H -2.014624 -0.466698 -1.304864
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 H -0.812967 -2.127896 -0.571302
 H 0.553646 -2.375001 0.081608
 H -0.679274 2.622986 0.323842
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 H 0.754769 1.033083 0.485324
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 H 1.240608 1.062162 -2.056094
 H 2.700559 0.916605 -0.307783
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 O 2.958054 -1.530015 0.208785
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 O -2.601825 -1.366145 -1.024293
 O 0.322800 -0.764907 1.462833
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 H 0.297593 2.501703 0.294055
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 H 2.926062 0.755237 1.479426
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 O 0.224708 1.851734 1.062014

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O 2.924725 0.887561 0.956833	H 2.739671 -1.346734 0.494431
O -2.956595 0.953723 -0.229540	H 2.833766 -0.712502 -0.901129
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H -2.684718 0.703318 0.679287	H 0.663612 2.623660 1.506152
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H 1.040850 0.609953 -1.609138	H -3.087810 1.264122 -0.318914
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 O 0.516021 0.131564 1.852244
 O 0.173363 -2.442522 0.976648
 H -1.070871 0.767708 -0.517367
 H -0.965835 0.863798 1.030999
 H 1.012282 0.562045 1.131664
 H 0.398447 -0.814717 1.581023
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 H 0.859713 -2.428709 0.272615
 H -3.037949 0.365378 0.448288
 H -3.650574 -0.706354 1.368731
 H 1.012311 0.993535 -0.965679
 H 1.203733 2.390441 -0.260092
 H -1.246826 -1.281909 -1.223348
 H -2.627505 -1.492794 -0.537334
 H 1.176940 -1.159382 -1.394399
 H 2.550219 -1.313062 -0.662179
 H 3.018019 0.596380 0.254092
 H 2.993535 -0.381626 1.423636
 H -0.866675 2.816479 0.085023
 O -0.315726 3.607116 -0.143040
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 H -0.285358 0.235551 -2.518797

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 O 0.562950 -1.091952 -1.328005
 H 1.054006 -1.526814 -2.031538
 O -2.095872 -1.254098 -1.695880
 O -3.150234 0.790603 -0.096770
 O -1.502607 -0.349747 1.830734
 H -1.254292 -1.208584 1.433212
 H -2.192446 0.026236 1.239989
 H -2.563182 1.569337 -0.166967
 H -2.842616 0.162916 -0.783732
 H -1.107265 -1.135017 -1.669875

H -2.241411	-1.989694	-1.089537	O 2.925003	-1.106035	1.468945
H -0.084709	-2.158735	-0.182520	H -0.705281	0.071109	-1.852723
H 0.317731	-2.739084	1.165447	H -1.654014	1.219699	-1.361801
H 0.775944	0.336410	-1.314341	H -1.802064	-1.501718	-0.901366
O 0.940198	1.372722	-1.183081	H -3.106119	-0.703881	-1.291944
H 1.164435	1.743718	-2.041185	H 0.023652	-1.086224	0.384845
O 2.213953	-1.248773	0.942979	H -0.719226	-0.656502	1.706450
H 1.851508	-0.506893	1.463727	H 1.528445	-0.989494	-1.318637
H 1.699139	-1.205834	0.105775	H 2.782950	-0.073345	-1.145974
O 3.768059	0.655545	-0.588488	H 3.327112	0.694723	0.750437
H 2.896567	1.051293	-0.743698	H 2.402966	1.764796	0.146768
H 3.550040	-0.085281	0.002888	H 0.236491	1.685176	-0.702344
O 0.787003	1.108138	1.742653	H 0.424219	0.997380	0.668942
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H -0.066976	0.604862	1.766178	H -2.536453	1.261098	0.974215
O -1.145294	2.773351	-0.008936	H -2.795223	-0.877988	0.830610
H -0.843630	2.665587	0.902763	H -3.306736	-0.860036	2.328545
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			H 1.978320	-0.995542	1.674124
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O -2.785211	-0.609105	-1.282161	oh.9h2o, E=	-764.023179	
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O -0.964204	0.583905	1.086360	O -2.456970	0.663448	1.162837
O -0.027280	0.235715	-1.413275	O -1.444296	-2.043129	1.259996
O 2.796936	0.007131	-1.619012	O 1.319399	-1.627168	1.614124
O 2.499528	-1.279571	0.949437	O 1.865214	0.854575	1.511624
O 0.463951	-2.195860	-0.408147	O 2.414548	0.699771	-1.335813
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H -3.142754	0.172310	-0.822183	H -1.648765	1.242155	1.315740
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H 1.698253	-1.692773	0.493601	H 2.249035	0.981799	0.629503
H 2.967765	-2.000200	1.379036	H 0.973757	1.425203	1.499195
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H -1.625503	-1.175086	1.311381	H -1.505630	-0.814283	-1.601694
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O -2.813474	-1.402823	-0.697077	O -2.528415	-0.628149	-1.270289
O -2.654765	-0.470279	1.740536	O -3.219041	1.958161	-0.141894
O 0.156308	-0.641950	1.286348	O -0.667037	1.531306	0.563750
O -2.355100	1.986397	0.351325	O 0.120709	0.077107	-1.445659
O 0.519966	1.869700	0.216914	O 2.562929	1.010324	-0.751144
O -0.975972	1.006168	-2.026146	O 3.548953	-1.576839	-0.108195
O 3.303294	1.393771	0.070168	O 0.899272	-1.968756	0.034866
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 O 3.532884 -0.858578 0.733098
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 O 2.480002 2.054739 0.348732
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 H 1.537641 -0.042971 -1.586079
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 H -0.186546 0.744020 -0.422096
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 H -2.870588 -1.324524 -0.692130
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 H 2.780423 2.934706 0.105488
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 H -1.715483 -1.222770 1.271347
 H -0.197052 -0.769832 -2.373873

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 O 1.179022 -0.929444 1.937814
 O 2.862458 -1.189101 -0.118848
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 H 2.122930 1.360477 -1.385191
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 O 1.230977 -2.362312 -1.405623

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 H 2.250900 0.167612 -1.084790
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 H 1.111233 -2.748297 0.124207
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 O 2.602969 -0.944085 -1.390584
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 H 2.459938 -1.788878 -0.924939
 H 1.470525 -2.194940 0.906349
 H 0.614158 -3.081046 0.016593
 H 0.260765 -0.489973 1.904354
 H 0.820505 -0.166381 0.512140
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 H -1.837858 -0.081560 1.612707
 H -1.460719 -1.537480 1.429515
 H 0.741619 1.607077 -0.921648
 H 1.987903 2.189368 -0.220102
 H 3.279858 0.361266 -0.239627
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 O -3.820673 0.045016 -0.098307
 O -1.841724 0.183914 1.915820
 O -0.575880 -2.000482 1.461255
 O 2.200678 -1.565532 1.366867
 O 2.395733 1.276714 1.402441
 O -0.174936 2.069241 1.252343
 H 2.249612 -0.348358 -1.470823
 H 2.853817 -1.666796 -2.110560
 H 2.324491 -1.615875 0.401969
 H 1.244258 -1.725577 1.489639
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 H 1.447806 1.579451 1.454060
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 H -1.328682 0.862001 -1.743468
 H 2.505186 1.325333 -0.334498
 H 1.432454 1.597703 -1.416323
 H -0.468095 3.007136 -1.528598
 H -0.245114 2.168640 -0.106880
 H -0.575506 -2.197530 -0.361927
 H 0.450882 -1.929814 -1.483225
 H -1.076118 -1.128593 1.660239
 H -0.891776 -2.649212 2.095576
 H 2.367325 0.311122 1.553396
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 H -1.211647 0.949213 1.696889

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 O 0.694649 1.730843 0.914899
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 O 1.692994 -0.725862 1.533680
 O 0.205203 -2.550195 -1.264761
 O 0.335225 1.021167 -1.778864

O 3.548410 1.845616 0.193603
 O 2.475803 -0.627577 -1.180545
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 H 0.397637 1.350950 -0.858375
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 H -2.215426 -1.005900 0.130475
 H -2.274618 -0.191446 1.451510
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 H 2.644951 2.091822 0.441504
 H 3.426014 1.083725 -0.394222
 H 0.992925 0.860199 1.256963
 H -0.196791 1.878324 1.283028
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 O -3.502005 -0.113792 0.115383
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 H 3.060948 0.994817 -1.845314
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 H -3.049221 0.093164 -0.740123
 H -1.566447 -0.675323 -1.983906
 H 2.015639 -2.061678 -0.285779
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 H 0.113432 -2.123282 -1.389666
 H 0.001785 2.467750 0.141789
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 H 3.257797 1.314606 1.418783
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oh.10h2o, E= -840.480735
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 H -1.455013 -1.503076 -1.281711
 H -0.277997 -1.810113 -3.065690
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 O -2.914199 -0.971426 -0.225452
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 O -0.814127 2.498751 0.474297
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H 1.889964 -1.860999 0.237482
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 O 0.635842 -0.385203 1.460875
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 H -2.421319 -0.530712 -1.449454
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H -1.230765	2.042789	-0.859346	H -0.636741	-2.330556	0.236361
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H 0.979915	1.465099	1.943759	H -1.598712	-0.190901	-2.086095
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O -2.203304	1.276481	0.828203	H 2.895197	0.707789	-1.267264
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oh.11h2o,	E=	-916.947309	H 0.069569	-0.190275	1.775714
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H 1.149072	1.141622	-1.400015	H 3.958560	0.045578	2.434721
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35

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