

# Electronic Supplementary Information for article:

## Infrared spectroscopy of $\text{O}^{\ominus}$ and $\text{OH}^-$ in water clusters: Evidence for fast interconversion between $\text{O}^{\ominus}$ and $\text{OH}^{\ominus}\text{OH}^-$

Jozef Lengyel, Milan Ončák, Andreas Herburger, Christian van der Linde,  
Martin K. Beyer\*

*Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens-Universität  
Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria.*

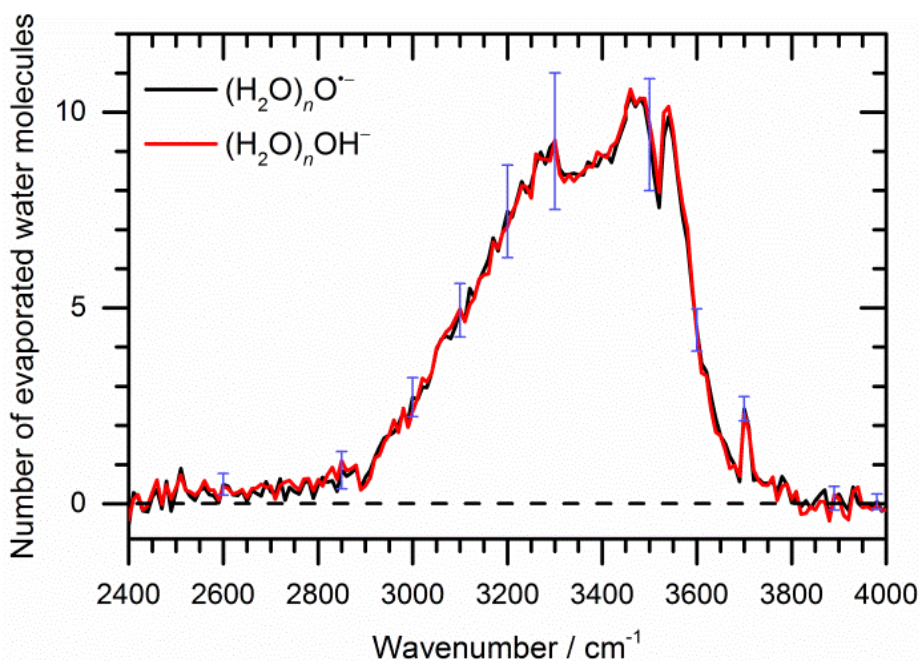
\* Corresponding author: martin.beyer@uibk.ac.at

### Experimental methods

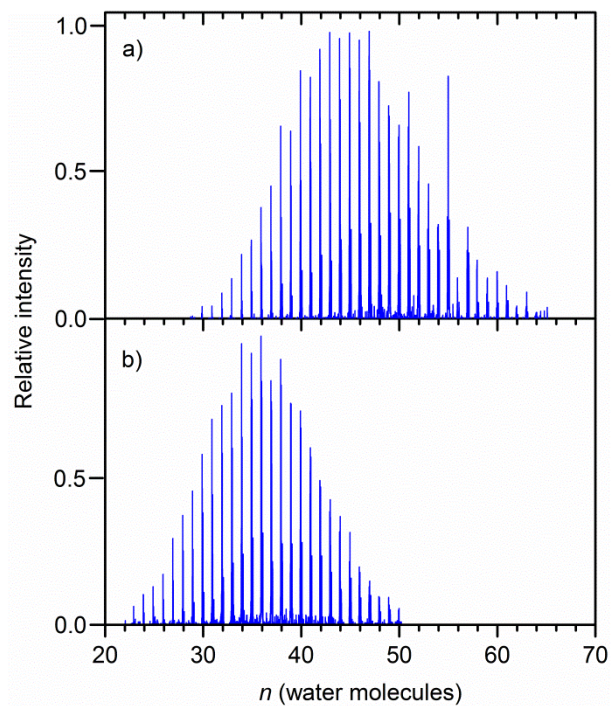
The IRMPD experiments are performed using a 4.7 T Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometer (Bruker/Spectrospin CMS47X) equipped with a tunable optical parametric oscillator (OPO; EKSPLA NT277). A detailed description of the FT-ICR can be found elsewhere.<sup>1,2</sup> The reactant ions,  $(\text{H}_2\text{O})_n^{\ominus}$ , 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.<sup>3,4</sup> 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  $8 \times 10^{-10}$  mbar, in which the ions are stored.  $\text{N}_2\text{O}$  is introduced through a leak valve at constant pressures at around  $1 \times 10^{-8}$  mbar. The reactions of anionic water clusters with  $\text{N}_2\text{O}$  produce both  $(\text{H}_2\text{O})_n\text{O}^{\ominus}$  and  $(\text{H}_2\text{O})_n\text{OH}^-$  product ions.<sup>5-7</sup> The reaction and the purity of product ions are monitored by recording mass spectra at different reaction delays.

$(\text{H}_2\text{O})_n\text{O}^{\ominus}$  and  $(\text{H}_2\text{O})_n\text{OH}^-$  clusters are irradiated at specific frequencies with tunable IR laser radiation. The laser radiation is introduced through a  $\text{CaF}_2$  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  $8\text{ cm}^{-1}$  for the IR radiation. The system offers tuning from 2400 to  $4000\text{ cm}^{-1}$  and produces pulses with energy of  $\sim 90\text{-}190\text{ }\mu\text{J}$ , 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  $(\text{H}_2\text{O})_n\text{O}^-$  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  $3520\text{ cm}^{-1}$ .



**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  $3500\text{ cm}^{-1}$ .

## Evaluating the relative probability of H<sub>2</sub>O and OH<sup>•</sup> evaporation

The relative activation energy of OH<sup>•</sup> evaporation with respect to H<sub>2</sub>O evaporation is derived based on the following observations and assumptions:

- 1) Within evaporation of 10 H<sub>2</sub>O molecules, there is a probability  $p_{\text{OH}^\bullet}$  of 2% to evaporate an OH<sup>•</sup> radical.
- 2) There are on average 46 water molecules per one OH<sup>•</sup> in the cluster.
- 3) We assume that the (H<sub>2</sub>O)<sub>*n*-1</sub>OH<sup>•</sup>OH<sup>-</sup> isomer is exclusively present.

In the experiment, 10 water molecules are being dissociated in the 3200–3500 cm<sup>-1</sup> region, see Figure S1. We can deduce the probability  $p_{\text{H}_2\text{O}}$  that in a specific evaporation event, H<sub>2</sub>O 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<sup>•</sup> radical,  $p_{\text{OH}^\bullet}$ , is equal to the ratio of dissociation rates of OH<sup>•</sup> and H<sub>2</sub>O,  $k_{\text{OH}^\bullet}$  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 (H<sub>2</sub>O)<sub>*n*-1</sub>OH<sup>•</sup>OH<sup>-</sup> and (H<sub>2</sub>O)<sub>*n*</sub>O<sup>-</sup> clusters are present in equal amount, i.e. 50%:50%. Then the ratio between the number of OH<sup>•</sup> and H<sub>2</sub>O is two times smaller, i.e.

there is on average one OH<sup>\*</sup> per 92 H<sub>2</sub>O water molecules. Equations (S3) and (S4) then change to:

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

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

Very small energy differences are sufficient to rationalize the preferential evaporation of H<sub>2</sub>O, 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 -0.353193 0.032018 -2.103294  
O -1.541575 1.701444 -0.606383  
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H 0.741661 -2.027698 0.136054  
H 1.260367 -1.190433 1.316482  
H -0.502807 -0.128858 2.117046  
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H 2.077700 -0.452079 -0.611622  
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H -0.713488 -1.236453 -1.375232  
H -1.164437 -2.783322 -1.302916

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o.7h2o, E= -610.430068  
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O 2.065050 -1.426672 0.641991

O 2.481426 1.063921 -0.588249  
O -2.477411 1.070216 -0.589661  
O -0.000544 -0.164301 2.090387  
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H -1.445459 -1.773716 -0.017299  
H -2.383985 -0.584525 0.236892  
H -1.662921 0.923728 -1.139036  
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H 1.439288 -1.777211 -0.018933  
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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.7h2o, E= -610.428228  
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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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O 0.191354 -1.684839 -1.457696  
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o.7h2o, E= -610.427784  
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O -1.095104 1.868668 -1.012004  
O -2.997375 0.131235 0.330758  
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H -2.513081 0.110681 1.167810

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o.7h2o, E= -610.427053  
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o.7h2o, E= -610.426573  
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H -2.879374 -0.224232 1.396198

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O 0.411539 -1.238434 -0.613670  
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H -2.429593 -0.670329 -1.400544  
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o.8h2o, E= -686.882410

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H 1.755695 0.747886 -1.175728  
H 3.128808 0.534641 -0.475269  
H 0.896004 -1.213567 -0.474472  
H 0.873723 -1.017883 1.051556  
H -1.369362 -0.878096 -1.571238  
H -2.800843 -0.534596 -1.045839  
H -0.940821 0.612396 0.851705  
H -1.163712 -0.766027 1.547940  
H -0.527539 1.286359 -1.190865  
H -0.325818 2.397360 -0.086547  
H 4.067923 -1.637546 -0.773604  
H 2.934254 -1.449493 0.258367  
H 0.765206 1.812508 1.707077  
H 1.714838 2.105254 0.515542  
H -3.248314 0.652562 0.917987  
H -2.662983 1.478743 -0.226965  
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H -1.883372 -2.164754 0.090514  
H -0.580286 -2.616398 0.768525

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o.9h2o, E= -763.345229  
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O 1.706605 1.528604 -0.430912  
O 3.470353 -0.245044 0.655931  
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O -3.786301 -0.224318 0.508923  
O 1.913537 -1.935941 -1.102778  
O -1.967418 -1.981871 -0.920848  
O 0.490445 0.204057 1.834475  
O 0.080362 -2.346388 0.943715  
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H -0.970385 0.959443 1.009090  
H 1.016351 0.622048 1.128131  
H 0.348524 -0.736668 1.553174  
H -0.737549 -2.336822 0.400517  
H 0.789348 -2.404979 0.265938  
H -3.048414 0.427665 0.431277  
H -3.641286 -0.644748 1.362714  
H 1.079823 0.968681 -0.983099  
H 1.262686 2.390811 -0.338074  
H -1.358764 -1.322862 -1.332980  
H -2.709759 -1.457491 -0.574164  
H 1.272137 -1.281967 -1.462675  
H 2.578737 -1.412356 -0.620325  
H 3.033528 0.539455 0.262598  
H 2.946847 -0.415683 1.448854  
H -0.813955 2.870424 -0.040110  
O -0.230478 3.620988 -0.310608  
H -0.442505 3.763604 -1.238520

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o.9h2o, E= -763.345158  
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O -2.024739 -1.696075 -0.429735  
O 1.526835 -2.153088 -0.977555  
O 0.956652 0.045496 1.411446  
O 1.897783 1.856148 -1.151258  
O 0.524777 2.728166 1.157865  
O -4.019667 0.138066 0.086891  
O -0.004017 -2.591114 1.397306  
O 3.426788 -0.294377 -0.024815

H 0.924860 -1.413096 -1.203870  
H 1.127807 -2.512419 -0.160346  
H -0.826667 -2.369235 0.923775  
H 0.303781 -1.729035 1.731978  
H 0.755006 -0.038474 0.463134  
H 0.779764 1.002815 1.577908  
H 2.958066 -1.043836 -0.448175  
H 2.881376 -0.144671 0.765319  
H -1.332237 -1.024661 -0.793189  
H -2.077808 -2.405195 -1.077634  
H 1.131428 1.278202 -1.343183  
H 2.587704 1.224392 -0.867576  
H -4.143075 0.499581 -0.796952  
H -3.390839 -0.605888 -0.043796  
H -0.379495 2.666018 0.787261  
H 1.101672 2.648751 0.368751  
O -1.833009 2.066773 -0.227949  
H -1.310086 1.388834 -0.719816  
H -2.539949 1.555749 0.197314

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o.9h2o, E= -763.344512  
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O -2.408033 -0.910197 1.196001  
O 0.239451 -1.851045 -1.608484  
O 2.525383 -0.523661 -1.307128  
O 1.465093 2.125405 -0.976170  
O -1.323450 1.859242 -1.349208  
O -1.952903 -0.600467 -1.647967  
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H 1.696804 1.839231 2.519941  
H 2.375126 -0.825642 0.403396  
H 1.333402 -1.553501 1.312026  
H 0.523178 2.058660 -1.223342  
H 1.459429 2.030720 -0.006836  
H -0.574028 1.578954 1.643601  
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  
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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  
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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.9h2o, E= -763.343567  
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O 1.878352 2.130457 0.042022  
O 2.640317 0.030504 -1.286246  
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  
H -2.848340 -1.407458 -0.341993  
H -3.114373 0.492494 0.837822  
H -4.216647 0.441797 -0.240677  
H -1.072345 1.118517 1.652552  
H -1.462835 1.762667 0.305085  
H 2.066095 -2.056099 0.852810  
H 2.595036 -0.912634 1.678610  
H 1.083711 0.971227 1.290810  
H 0.464642 -0.469209 1.340147  
O 0.315283 -1.986645 0.325663  
H 0.327162 -1.533980 -0.578315  
H -0.597606 -2.326779 0.336071

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o.9h2o, E= -763.343182  
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O 1.492804 2.001876 0.036234  
O -0.293098 0.463432 1.328894  
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  
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H 0.898486 2.032843 -0.749878  
H -2.157236 -0.115946 1.310328  
H -3.160316 -0.942607 0.474994  
H -1.894697 -1.919444 -0.959199  
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H 0.433576 -1.408368 -1.019920  
H -0.435180 -0.593035 -0.005229  
H -1.170347 2.042679 -1.279039  
H -0.492808 0.757466 -1.777145  
H 2.671791 -1.329000 -0.915506  
H 1.984487 -2.036378 0.217398  
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H -2.818899 1.652888 0.368534

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o.9h2o, E= -763.341708  
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O 0.717777 1.870189 -0.440335  
O 0.904227 -0.462911 -1.588189  
O -1.372930 2.248004 1.235086  
O -1.195458 -0.239640 2.292770  
O -2.216957 -2.074628 0.680416  
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  
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H -0.113858 -2.359045 0.776484  
H -1.964063 2.116635 0.468889  
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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  
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H -1.994144 -1.332732 1.312960  
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o.9h2o, E= -763.341138  
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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  
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O 3.111825 -0.813607 -0.508294

O 2.974261 2.187397 -0.078464  
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H 2.736528 -0.796695 0.384848  
H 2.024988 2.025157 0.057603  
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H 0.771253 -1.865478 0.586848  
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H -1.349690 0.196164 -2.205195

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o.9h2o, E= -763.341019  
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O 0.893394 0.513801 1.787394  
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  
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O 1.890101 -1.908112 -0.801129  
O 3.416516 -0.645198 1.241165  
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H -1.994338 -0.601177 1.376213  
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H 0.436632 0.759159 2.597360  
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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  
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H -1.722206 0.823299 -1.312501  
H -2.520070 1.403933 0.645940  
H -1.452377 2.398980 0.067660  
H 3.008330 -1.334551 0.681017  
H 2.641864 -0.204827 1.634959

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o.9h2o, E= -763.340353  
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O 0.244563 -2.004623 -0.444286  
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  
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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 -1.592264 -2.157854 -0.678637  
H -0.789335 1.028241 -1.658666  
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H 1.760125 0.716756 -1.762044  
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H 2.045305 -1.628501 -0.138267  
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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.9h2o, E= -763.339953  
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H -1.952875 0.170339 -1.574073  
H 0.145477 1.133258 -1.655643  
H 0.151245 -0.414321 -1.509828  
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o.10h2o, E= -839.808945  
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O 2.587497 -0.095623 -1.715382  
O -3.233746 2.060653 -0.382178  
O 0.576023 -2.275215 0.377646  
O -0.588322 -0.117578 1.593060  
O -2.177389 -2.211253 -0.766064  
O -3.260714 -0.425957 1.050770

O 3.077201 -1.226987 0.783265  
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H 1.662077 -0.410580 -1.875056  
H 1.970502 1.641049 1.240441  
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H -1.566889 -0.237757 1.622134  
H -0.219357 -0.960973 1.227447  
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 -3.016822 -1.088224 0.363980  
H 1.824067 3.341305 -0.753162

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o.10h2o, E= -839.808218  
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O 1.121618 1.734282 2.018324  
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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 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  
H -0.168633 2.475173 -0.749495  
H -0.105232 -1.348465 -1.758113  
H 1.169183 -2.029075 -1.133687  
H 0.250482 1.298871 2.123901  
H 1.011471 2.246325 1.185517  
H -1.418879 -1.979504 0.134722  
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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  
H -2.660030 1.599792 -0.801797

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o.10h2o, E= -839.807687  
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O 0.138858 2.437555 -0.309374  
O -3.057597 0.732620 -1.108091

O 2.463745 1.767492 0.667335  
O 2.673362 0.168964 -1.643157  
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O -3.113058 -1.659709 0.276046  
O 2.442214 -2.203030 -0.092075  
O 1.732992 -0.632697 2.060255  
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O -1.931020 1.797617 1.273046  
H -2.155948 0.650609 -1.455721  
H -0.432588 -0.096305 -2.907490  
H -2.574936 -2.271902 -0.241520  
H 0.704483 -2.247045 -0.438133  
H 2.793071 0.764009 -0.878884  
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H -2.828325 -2.202963 -0.380995  
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o.11h2o, E= -916.268753  
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H 1.707638 -2.042485 0.521705  
H -2.291654 -1.538567 -0.348716  
H -1.365403 -1.575556 1.521623

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o.11h2o, E= -916.268314  
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o.11h2o, E= -916.266390  
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O 1.057837 1.779007 0.134827  
O 2.587925 -1.178649 -1.739556  
O 0.324478 -2.236810 -0.373786  
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O -0.924114 3.629077 -0.052942  
H -0.108508 3.083117 0.072309

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o.11h2o, E= -916.266202  
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O 3.719065 0.259310 -0.708835  
O 1.714436 -1.716673 -1.000065  
O 2.504231 0.804308 1.741565  
O -0.194640 1.385312 0.841114  
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O -1.191029 -0.821316 2.178112  
H -1.836815 -1.209807 1.500040  
H -1.644991 -0.812569 3.025075  
H -3.077816 -0.890040 -0.108771  
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H 3.049311 0.658307 0.935552  
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H 1.579593 -1.802745 -0.025928  
H 1.102100 -1.010689 -1.292742  
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o.11h2o, E= -916.265120  
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H 2.662707 1.678235 0.915518  
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O 1.091480 2.179790 -1.084059  
O 3.641833 1.134166 -0.664582  
O 2.465908 -1.188975 -1.474995  
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H -2.675195 -3.565774 -1.150908  
H 0.569342 -1.434313 -1.302242  
H -0.282674 -1.583674 -0.026494  
H 1.194770 3.347934 -0.557535  
H 0.210614 3.200298 0.563908  
H 1.856539 0.297957 -0.662543  
H 2.725442 -0.691501 -1.380571  
H -0.875715 1.082818 0.715859  
H -2.113083 1.930946 0.267338  
H -3.659957 0.549967 0.605749  
H -4.150149 1.766583 1.431777  
O 0.477896 2.285235 -2.077474  
H -0.217167 2.033577 -1.437868  
H 0.995759 1.477895 -2.216995

34  
o.11h2o, E= -916.261304  
O 1.461358 -0.222412 -2.620273  
O 3.299602 1.079452 -0.889756  
O 1.200931 1.590897 0.899983  
O -0.369496 0.078383 -0.610773  
O 0.380495 -1.926483 1.000324  
O -1.909865 -3.487596 0.751937  
O -2.621567 -1.477694 -0.848756  
O -4.040050 0.736856 0.125288  
O -1.990528 2.251027 -0.768021  
O -0.450031 3.701821 1.100468

O 2.304232 -0.541768 2.311874  
H 0.596393 -0.050328 -2.203546  
H 2.056724 0.447077 -2.229110  
H 3.364914 0.147876 -0.618582  
H 2.642126 1.448541 -0.265809  
H 0.597573 1.015166 0.338209  
H 1.568840 0.984117 1.577350  
H -1.774681 -0.981959 -0.941337  
H -3.262377 -0.797012 -0.556137  
H -3.360843 1.375336 -0.217194  
H -3.875633 0.700504 1.072850  
H -1.563184 2.831161 -0.105986  
H -1.328794 1.542188 -0.938860  
H 1.545389 -1.122665 2.079615  
H 2.952082 -0.767128 1.631292  
H 0.200800 2.959109 1.177014  
H 0.023736 4.389950 0.623348  
H 0.028285 -1.188496 0.427773  
H -0.343288 -2.583723 1.059842  
H -2.284649 -2.752976 0.191412  
H -1.763682 -4.210456 0.134280  
H 1.941068 -2.038113 -0.009347  
O 2.704199 -1.767486 -0.557135  
H 2.284965 -1.468144 -1.388347

34

o.11h2o, E= -916.260402  
O 0.399931 -0.282551 -0.790548  
O 2.289487 0.754911 0.872753  
O -0.347289 2.509089 -1.095637  
O 0.399042 2.721985 1.624365  
O 2.706712 -1.538008 -1.546659  
O 1.356392 -1.991688 1.149251  
O -1.261760 0.492050 1.332414  
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  
H 1.661825 0.617491 0.129746  
H 3.166122 0.750027 0.437468  
H 0.830795 -1.726301 0.371886  
H 1.790786 -1.153058 1.390348  
H -1.007374 -1.520800 -0.874647  
H -2.542151 -1.645676 -1.045110  
H -0.757809 0.240552 0.525740  
H -1.421698 -0.367665 1.781688  
H -0.032679 1.586012 -1.129090  
H -0.077802 2.798647 -0.198581  
H 1.838904 -1.066056 -1.439990  
H 2.694472 -2.165297 -0.811523  
H -0.252357 2.014112 1.793975  
H 1.234397 2.228266 1.543877  
H -4.686495 -0.656235 -1.018993  
H -3.553112 0.371562 -1.242966  
H -2.580723 1.358442 0.352428  
H -2.166282 2.169783 -0.856979  
H -0.470936 -2.310490 2.032168  
H -1.668607 -2.312454 1.070810  
O 4.459985 0.400158 -0.855653  
H 4.421305 1.067697 -1.547537  
H 3.910537 -0.353818 -1.191555

19

oh2.6h2o, E= -533.967377  
O 0.285834 -0.443151 -1.587703  
O 2.028998 1.237601 -0.475929  
O -1.882484 -1.502281 -0.081664  
O -0.159188 -0.733878 2.046989  
O 1.674403 -1.815175 0.038469  
O -1.777207 1.231784 -0.957751  
O -0.141408 1.936260 1.198000  
H 0.405310 -0.654263 -2.517857  
H -1.168388 -1.313370 -0.724689  
H -1.442491 -1.325663 0.774171  
H -0.168937 0.231340 1.858089  
H 0.583238 -1.079924 1.521039  
H 1.075652 -1.353279 -0.684979  
H -0.997470 0.751105 -1.334628  
H -2.259605 0.483123 -0.568307  
H 1.385844 0.684816 -1.010041  
H 2.491798 0.578869 0.054035  
H 0.690537 1.873464 0.687752  
H -0.827067 1.834501 0.502125

19

oh2.6h2o, E= -533.966040  
O 0.249376 0.785340 -1.403067  
O -1.358657 2.183304 0.026048  
O 2.331372 1.166696 0.182482  
O -1.680394 -0.200620 1.624283  
O 1.053164 -0.854774 1.729865  
O -1.817639 -1.165450 -1.037599  
O 0.967179 -1.784249 -0.918195  
H -1.240927 -0.429003 -1.325946  
H -1.931368 -0.975068 -0.083799  
H 0.846076 -0.837751 -1.191917  
H 0.041267 -2.079535 -0.956659  
H 1.547337 1.109712 -0.446974  
H 2.929415 0.483120 -0.137052  
H -1.629291 0.696893 1.245359  
H -0.743448 -0.447392 1.782168  
H 1.484390 -0.021404 1.461017  
H 1.056906 -1.357089 0.886665  
H -0.695279 1.661466 -0.581822  
H 0.379717 1.154069 -2.281566

19

oh2.6h2o, E= -533.964251  
O -0.050762 1.406585 0.905680  
O 2.527160 1.438951 -0.110267  
O 2.107757 -1.497269 -0.048949  
O 0.240348 -0.152598 -1.597189  
O -0.300047 -1.248264 1.552830  
O -1.957957 -1.057335 -0.523924  
H 1.649712 1.583088 0.306987  
H -0.113686 0.497245 1.292305  
H 0.535809 -1.540522 1.147335  
H -0.979437 -1.328589 0.824458  
H -2.585851 -1.715648 -0.829892  
H -2.467760 0.256697 -0.291478  
H 1.473847 -1.178123 -0.731262  
H 2.527549 -0.667779 0.227416  
H -0.618450 -0.631638 -1.385687  
H 0.196129 0.551644 -0.929816

H 2.304878 1.178911 -1.011902  
H -0.964494 1.587582 0.595305  
O -2.686281 1.285821 -0.079902

19

oh2.6h2o, E= -533.963373  
O -0.682912 -1.518390 -1.060884  
O 1.953792 -1.770954 0.035739  
O 2.920787 0.855968 -0.341262  
O 0.701320 1.673783 0.480992  
O -0.315817 -0.471240 1.535791  
O -2.997707 -0.066490 0.469669  
O -1.310509 1.291289 -1.212958  
H -0.631643 -1.188695 -0.137747  
H 0.231754 -1.823849 -1.176892  
H 1.322246 -1.551713 0.737968  
H 2.373671 -0.907908 -0.171287  
H 1.995960 1.270689 -0.009334  
H 0.085542 0.407901 1.228078  
H -1.273096 -0.309327 1.565559  
H -2.497674 0.568402 -0.103571  
H -2.888224 -0.899564 -0.004242  
H -1.025779 0.419800 -1.537342  
H -0.553131 1.558834 -0.613000  
H 0.708751 2.503701 0.965122

19

oh2.6h2o, E= -533.962901  
O 0.648718 -0.847015 -0.964572  
O -1.447946 1.038290 -1.249956  
O -0.290680 1.846746 1.254236  
O -0.598032 -0.984520 1.283242  
O 2.907776 -1.435791 0.143964  
O -3.144340 -0.970089 -0.108639  
O 2.017310 1.405720 -0.352316  
H 0.383821 -1.449417 -1.665284  
H -0.079897 -1.566656 1.845845  
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  
O -1.263634 1.815619 -0.554178  
O -3.558610 -0.067344 0.121664  
O 2.048511 -1.821741 -0.153661  
O 0.825437 1.850819 1.336638  
O 0.484913 -0.836503 1.991072  
H 0.012404 -0.392367 -2.550114  
H 1.607386 0.678089 -1.228329  
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

H -0.186672 2.093346 0.267688  
H -1.901051 -0.338654 1.074004  
H -2.098270 1.013870 -0.743598  
H -1.713801 -0.470850 -1.077024  
H -0.300280 0.772577 1.885539  
H 1.175229 1.004661 1.438751  
H -0.779528 -1.267349 1.580777  
H 1.246347 -1.685876 0.749896

22

oh2.7h2o, E= -610.425035  
O 0.157363 -0.154279 -1.704503  
O -1.193921 1.558121 -0.364097  
O -1.198669 -1.877996 -0.194719  
O 1.917823 -1.766458 -0.551087  
O -3.393196 0.192344 0.314480  
O 1.605894 2.030494 -0.588991  
O -0.444139 -0.108471 1.871787  
O 2.334427 0.185106 1.439516  
H 0.047524 -0.210049 -2.657016  
H 1.350024 -1.141089 -1.089280  
H 1.260364 -2.345736 -0.148432  
H -0.739463 0.877697 -0.980205  
H -0.476248 2.198135 -0.227391  
H -0.739763 -1.285511 -0.859442  
H -2.089975 -1.506914 -0.120649  
H 1.273749 1.298431 -1.148667  
H 1.983197 1.550947 0.176961  
H 2.378713 -0.536291 0.778072  
H 1.418463 0.103845 1.773973  
H -0.691236 0.602197 1.252452  
H -0.620945 -0.902878 1.328560  
H -2.639060 0.826316 0.141975

22

oh2.7h2o, E= -610.423110  
O 0.822569 1.959700 0.078505  
O -1.978465 1.739805 -0.000476  
O -2.371779 -0.564862 -1.594348  
O -2.280331 -0.591044 1.674494  
O -0.519481 -1.514484 0.057885  
O 1.344674 -0.307688 1.677615  
O 3.580755 -0.352650 -0.177102  
O 1.278262 -0.242918 -1.589217  
H 0.988810 1.299165 0.784066  
H -0.154964 2.029836 0.042554  
H -2.101190 1.147019 0.764150  
H -2.100479 1.121889 -0.748660  
H -1.626021 -0.987482 -1.073457  
H -3.164756 -0.855036 -1.132042  
H 0.684603 -0.814750 1.143399  
H 2.194128 -0.480663 1.236307  
H 2.807237 -0.421759 -0.797758  
H 3.694723 0.598926 -0.079152  
H 1.090752 0.649751 -1.228238  
H 0.633277 -0.803072 -1.092341  
H -1.530068 -1.019225 1.096378  
H -0.425690 -2.471479 0.065952

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  
O -0.521286 1.120904 -1.084933  
O -0.909898 -3.034550 -0.194418  
O -2.100097 -0.551025 0.065073  
O 0.250786 -0.952994 1.695616  
O -2.538396 2.437801 0.021337  
O 1.234837 1.806531 0.894419  
O 3.475114 0.452059 -0.288562  
H 0.804684 -0.985413 0.890590  
H -0.627849 -0.734985 1.332754  
H -1.561426 -2.307032 -0.183570  
H -1.526932 0.038269 -0.527116  
H 0.529651 -0.241991 -1.119817  
H -0.470764 1.429352 -1.993680  
H 0.979052 1.087636 1.490613  
H 0.635190 1.681450 0.119007  
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 1.483959 0.696920 -1.249846  
H 2.745565 0.675386 -0.343459  
H 2.549237 -1.372069 0.680899  
H 0.700187 -1.105718 -0.489609  
H 0.289526 -2.297891 0.440157  
H -1.009044 0.780803 -1.524704  
H -2.247481 0.962532 -0.615707  
H -1.908607 -0.012846 1.380882  
H -3.477758 -0.054495 1.518276  
H -0.181218 1.173593 1.596651  
H 0.134554 -0.352883 1.542557  
H -1.124831 -1.657488 -1.207811  
H -2.217090 -1.746768 -0.144405  
H 0.971178 2.258788 0.127081  
H -0.549336 2.336773 -0.106162  
H 0.463744 -0.727622 -2.543181

25  
oh2.8h2o, E= -686.886503  
O 0.288145 -1.624151 0.238998  
O 2.218250 -0.865623 -1.093170  
O 0.779885 0.680709 1.473870  
O 3.685440 0.080679 0.916845  
O -1.883971 -1.415021 -1.430812  
O 1.046911 1.693333 -1.155772  
O -1.724093 1.397772 -1.502387  
O -1.959852 1.550325 1.267819  
O -2.365947 -1.221121 1.387589  
H -1.434807 -1.392883 1.155392  
H -2.390008 -0.242826 1.456421  
H -2.481733 -1.419941 -0.663415  
H -1.022479 -1.575756 -0.977580  
H 0.913708 1.556673 -0.196906  
H 1.486635 0.860814 -1.408500  
H 1.367645 -1.268942 -0.553238  
H 2.442951 -1.463046 -1.810588  
H -1.809951 0.426029 -1.606830  
H -0.761210 1.566603 -1.553121  
H -1.953499 1.592589 0.283353  
H -1.023143 1.469106 1.509842  
H 3.229522 -0.289465 0.097728  
H 0.559742 -0.225488 1.111093  
H 1.731843 0.648566 1.646987  
H 0.466648 -2.457259 0.685522

25  
oh2.8h2o, E= -686.885921  
O -1.245513 -1.680884 -0.081399  
O -2.340051 -0.000501 1.938301  
O 0.407353 -0.734818 1.641777  
O 0.714724 -0.921938 -1.719835  
O -2.289736 -0.028425 -1.852708  
O -1.988687 2.058073 -0.012274  
O 2.806556 -1.291599 0.252180  
O 3.458261 1.612467 -0.010165  
O 0.797077 1.302241 -0.134385  
H -1.491735 -2.609079 -0.081441  
H -2.025334 -0.719646 -1.174753  
H -1.513578 0.012613 -2.423262  
H -0.191996 -1.229789 0.977328  
H -0.257160 -0.395441 2.263044  
H -0.014757 -1.334177 -1.172479

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  
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H -0.214700 -0.881307 1.107463  
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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

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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  
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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

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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  
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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  
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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  
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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  
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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  
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H 0.510256 -0.513863 1.658501  
H -0.820226 0.337932 1.511718  
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H 2.359536 -1.934672 0.092095  
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H 1.126357 2.435821 -0.530955  
H -1.671586 -2.543514 -0.367865  
H -1.646109 -1.753328 0.937757  
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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  
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O -0.467553 1.393605 -1.874683  
O -0.069903 -1.200316 -1.884208  
H -2.438353 -0.079498 -0.079690  
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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  
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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  
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H -3.426743 1.502807 -0.097893  
H 1.864133 1.779976 -0.171727  
H -2.281090 -0.952989 0.294163  
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H -1.298247 1.244955 1.509061  
H 0.568456 1.952259 0.690894  
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oh2.8h2o, E= -686.883558  
O 0.291468 0.076125 1.580604  
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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  
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H 1.229330 -1.342891 -1.158720  
H 1.377284 -0.891746 0.982929  
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H 0.528062 0.973390 0.248406  
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oh2.8h2o, E= -686.882925  
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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  
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H 2.461862 -0.901569 1.082614  
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H -3.096006 1.128132 0.141377  
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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

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oh2.8h2o, E= -686.882591  
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O 2.353121 -1.388725 1.484722  
O -0.509075 -0.617311 1.544185  
O -0.607855 1.961466 -0.719220  
O 2.365697 1.487059 -1.063482  
O 2.162392 -1.352030 -1.377752  
O -2.766081 0.964196 0.834758  
O -3.267891 -1.305267 -0.855198  
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H 2.081652 -0.448245 1.489834  
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H 1.186636 -1.323362 -1.413145  
H -0.516864 -0.798554 -0.109453  
H -0.582476 0.170173 -1.285953  
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oh2.8h2o, E= -686.880694  
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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  
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O 0.424805 -1.497421 1.921964  
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H 0.380006 -1.403619 -2.788194  
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H 0.407856 -0.495166 1.975621  
H 0.459641 -1.815657 2.827564  
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H 1.869826 -1.568823 0.518837  
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oh2.9h2o, E= -763.349130  
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O -1.659024 -1.690339 1.418405  
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O 1.122319 -2.222083 1.002113  
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O 2.198491 0.476239 -1.338426  
O -1.573852 -1.450749 -1.420005  
O -2.097306 1.087767 -1.294309  
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H 0.193061 -2.106697 1.265017  
H -1.890600 0.099040 -1.401766  
H -2.792840 1.294064 -1.923926  
H -2.228430 -2.083502 2.084602  
H -1.749780 -0.692043 1.515808  
H 1.690159 -0.482561 -1.520862  
H 1.392193 -2.324467 -2.194998  
H 1.031680 1.868901 -1.388107  
H -1.704526 -1.740250 -0.499820  
H -0.578143 -1.570188 -1.587319

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oh2.9h2o, E= -763.348650  
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O 0.314136 -2.128167 -0.603402  
O 0.660084 -0.142763 -2.150990  
O 0.396929 -1.519421 2.087174  
O -1.013543 0.828391 2.126404  
O 0.369606 2.559537 0.777711  
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H -1.223532 -2.205394 -0.663513  
H -0.570350 1.160074 -1.818090  
H -0.651937 2.292135 -0.781679  
H 1.336855 -1.282604 1.997414  
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H 1.847114 1.840775 -0.088128  
H 2.030045 -1.527506 0.066571  
H 2.844239 -0.242637 0.253595  
H 0.528439 -0.984185 -1.560811  
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oh2.9h2o, E= -763.347814  
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O -1.032966 -2.096451 1.518334  
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O 1.799451 -1.797321 1.147954  
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H -3.184772 0.365855 -1.776799  
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H 1.654729 -0.073634 -1.545886  
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H 0.381008 1.956318 -1.391619  
H 2.525705 1.143370 -2.179395  
H -1.307834 -2.273963 -0.422903  
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oh2.9h2o, E= -763.346505  
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O -1.857887 1.716694 -0.523257  
O 3.192729 -0.525592 0.292074  
O 1.162565 -1.195840 -1.394820  
O -1.450076 -1.048462 -2.019011  
O -3.051877 -0.805046 0.219606  
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O 0.760822 1.473744 -1.766902  
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H 1.648984 1.961416 -0.237847  
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H 0.421846 1.735152 1.471477  
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H -1.349752 1.714406 0.359418  
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H -0.420598 -1.553647 1.804667  
H -1.867876 -1.037748 1.595190  
H -2.553267 -1.167797 -0.544257  
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oh2.9h2o, E= -763.346319  
O -0.128508 -0.001338 -1.613396  
O 1.611785 1.577820 -0.497782  
O -1.532087 1.219168 0.186012  
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O -0.476677 3.670792 -0.162911  
O 0.493607 0.267755 1.815383  
O -1.799918 -2.024747 -0.779600  
O 1.898837 -1.808438 -1.053667  
O 0.232353 -2.352272 1.083416  
H -1.076299 0.754724 -0.602564  
H -0.984940 0.906973 0.943811  
H 0.995313 0.664753 1.079822  
H 0.408094 -0.697562 1.602305  
H -0.598821 -2.366003 0.560341  
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H 1.172817 2.437308 -0.410111  
H -1.210312 -1.336974 -1.177042  
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H 3.007897 -0.220064 1.414148  
H -0.981343 2.807456 -0.020487  
H -0.282340 0.158069 -2.548752

28

oh2.9h2o, E= -763.346230  
O 0.115707 -0.045781 -1.483025  
O 1.819513 1.101959 0.091959  
O -1.400894 1.444107 0.057456  
O 4.035635 -0.326034 0.065580  
O -3.832065 0.224749 0.002242  
O 0.344900 3.525987 -0.130065  
O -0.072288 0.176805 2.056590  
O -1.956844 -1.776153 -0.996290  
O 1.691996 -2.131993 -0.664042  
O -0.370637 -2.415319 1.205101  
H -0.909625 0.906436 -0.641521  
H -1.052756 1.037252 0.892877  
H 0.749139 0.418944 1.591422  
H -0.199337 -0.782903 1.849763  
H -1.057113 -2.314031 0.509873  
H 0.452773 -2.481226 0.677200  
H -3.022949 0.793780 0.004336  
H -3.868061 -0.131807 0.895791  
H 1.192759 0.668926 -0.585473  
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

28

oh2.9h2o, E= -763.346181  
O -0.242811 -0.042611 -1.543010  
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  
O 0.395793 0.272828 -1.529136  
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  
O -0.533433 1.763153 -1.784977  
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  
O -2.362155 0.333486 -1.744752  
O -2.572683 -2.109793 -0.471260  
O 0.302529 0.094290 -1.036473  
O -0.354295 1.415351 1.189566  
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  
H 0.952550 2.318302 0.661849

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oh2.9h2o, E= -763.342945  
O -1.439022 -1.488343 -1.002728  
O 1.088728 -2.032959 -0.955851  
O -1.193522 -1.999330 1.718271  
O 2.081071 0.195920 -1.795836  
O -0.714391 0.779016 -2.237626  
O -2.901753 0.073504 0.648799  
O -1.539605 2.304941 -0.140019  
O 0.435566 2.934748 1.415177  
O 2.412139 1.037313 0.824098  
O 1.624260 -1.323345 1.752768  
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  
H 2.752772 0.044542 -2.465794  
H 1.734083 -0.719352 -1.512344  
H -0.273762 -1.728419 1.867674

H -1.292189 -1.975848 0.737266  
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  
O 0.149100 0.534927 1.950097  
O -0.352430 2.506549 0.211474  
O -2.185398 -0.473199 0.996259  
O -2.808603 1.528428 -0.813375  
O -1.623178 -2.486720 -1.115713  
O 0.952980 -1.959546 -0.780969  
O 0.668947 -1.999965 1.910695  
O 2.744669 -0.015046 -1.561773  
H 1.992401 0.394728 -2.020723  
H 2.758262 0.469222 -0.702753  
H 0.522157 -0.998015 2.005831  
H -0.205751 -2.376276 2.054367  
H 1.729527 -1.436013 -1.082258  
H 0.980067 -2.004953 0.206782  
H 0.059609 0.856112 2.852300  
H 1.950534 2.230243 0.408487  
H 1.647127 1.019874 1.285623  
O 2.382639 1.440848 0.758251  
H -1.300674 2.490012 -0.016311  
H -0.249760 1.824555 0.931662  
H -1.331207 -0.118942 1.363078  
H -1.965835 -1.205971 0.398580  
H -0.632363 -2.331734 -1.158206  
H -2.211209 1.215614 -1.508508  
H -2.742482 0.818541 -0.133774  
O -0.054535 0.669637 -1.850366  
H 0.038019 -0.171433 -1.375265  
H -0.031948 1.357125 -1.145554

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oh2.9h2o, E= -763.340703  
O 0.865542 2.771761 -0.377494  
O -1.299189 1.330095 -1.102798  
O -2.625042 -0.129347 0.577832  
O 0.031053 -0.999077 -1.264974  
O -1.995289 2.906051 0.898005  
O -0.644218 -1.844061 1.457536  
O 3.034842 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  
H -1.513897 -2.202348 -1.235697  
H -2.156688 0.396222 -0.153607  
H -1.707779 1.535115 -1.948413  
H -0.389735 -0.096583 -1.305934



H 0.098105 -1.174652 -0.311815  
H 2.291864 1.766334 0.128570  
H 2.681145 0.550035 1.025421  
H 1.945920 -1.101893 -1.469323  
H 3.082511 -0.262096 -0.862859  
H 1.239096 -1.522383 1.640659  
H 2.457284 -1.527207 0.677845  
H -1.756456 2.365633 0.065128

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oh2.9h2o, E= -763.340523  
O -3.613684 -1.453302 0.165392  
O -3.154282 1.154381 -0.238979  
O -0.902824 1.142274 1.108920  
O -0.811286 -1.394146 0.250228  
O -0.307979 1.858901 -1.067760  
O 1.578495 0.589924 2.210396  
O 1.773027 -1.876797 1.096929  
O 2.811864 -0.909100 -1.121975  
O 2.379120 1.770880 -0.204420  
O 0.192021 -0.709856 -2.221602  
H -3.949068 -1.418127 1.066614  
H -3.530699 -0.495977 -0.098678  
H -2.731837 1.432508 -1.061717  
H -2.365565 1.198973 0.388093  
H -0.775395 -0.443182 0.536752  
H -0.225949 -1.132283 -1.441411  
H 1.145112 -0.795638 -2.046384  
H 2.469811 -1.337720 -0.278041  
H 3.594694 -1.399819 -1.384824  
H 1.778106 -1.048484 1.643848  
H 0.827271 -1.970851 0.862491  
H 1.460551 1.912619 -0.527632  
H 2.657847 0.940148 -0.626948  
H 0.623976 0.723994 2.001884  
H 2.006657 1.090504 1.482509  
H -0.563370 2.015823 0.880203  
H -0.214805 0.961358 -1.462203  
H -1.763109 -1.619120 0.248413

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oh2.10h2o, E= -839.809614  
O -1.798360 -2.326206 -0.745013  
O 0.594025 -1.243495 -0.766971  
O 0.055406 0.978854 -1.827368  
O -2.509119 0.154134 -1.712364  
O -1.919032 -1.324277 1.996262  
O 2.107785 2.221362 -0.514598  
O -3.121563 1.000406 0.882859  
O -0.630434 2.141093 0.544229  
O 0.557124 -0.032177 1.690039  
O 3.199087 -1.983233 -0.570162  
H 2.258123 -1.758461 -0.780688  
H 3.141065 -2.778674 -0.032012  
H -0.833223 -2.013456 -0.819234  
H 0.580178 -0.883193 0.153829  
H -2.476654 -0.811041 -1.786798  
H -1.563298 0.467426 -1.795865  
H -1.931794 -1.854637 1.182180  
H -1.006875 -0.982489 2.060488  
H 1.535815 0.080826 1.720342  
H 0.184436 0.826392 1.365179

H 1.534786 2.709649 0.090522  
H 1.447944 1.734223 -1.075854  
H 0.448002 -0.387681 -1.333113  
H 0.179776 1.237052 -2.744390  
H -1.566556 1.923333 0.757406  
H -0.514082 1.859661 -0.393098  
H -3.076236 0.700349 -0.049449  
H -2.829235 0.218024 1.392100  
O 3.230108 0.307946 1.146706  
H 3.390004 -0.468006 0.577098  
H 2.977612 1.025440 0.522397

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oh2.10h2o, E= -839.807519  
O 2.262515 -1.223238 -1.489316  
O 2.218220 1.366357 -1.309536  
O 2.277731 1.402801 1.402997  
O -0.348922 2.018450 1.258205  
O -1.867393 0.020986 1.923388  
O -0.451628 -2.078753 1.440116  
O -0.423104 2.079055 -1.194048  
O -0.371915 -2.180064 -1.355863  
O -2.004270 -0.029977 -1.909524  
O -3.937707 -0.038187 -0.128578  
O 2.287815 -1.442527 1.351118  
H 2.245142 -0.208472 -1.481426  
H 2.929453 -1.483277 -2.129968  
H 2.406683 -1.480760 0.384999  
H 1.350135 -1.683222 1.483003  
H -1.427088 0.742352 -1.697195  
H -3.217731 -0.044794 -0.855715  
H 1.311789 1.635433 1.457998  
H -0.555584 2.832090 1.726689  
H -1.433684 -0.824229 -1.783518  
H 2.380801 1.473379 -0.335147  
H 1.285528 1.668634 -1.410827  
H -0.701460 2.937922 -1.522733  
H -0.426494 2.117963 -0.093372  
H -0.448864 -2.250415 -0.383652  
H 0.549497 -1.892029 -1.505545  
H -1.011448 -1.250982 1.642906  
H -0.769518 -2.771364 2.025293  
H 2.319928 0.436483 1.547749  
H -2.626821 0.057072 1.315110  
H -1.290986 0.828989 1.703686

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oh2.10h2o, E= -839.805688  
O 3.968600 -0.363636 -0.644166  
O 2.238005 0.236993 1.599060  
O 0.843201 -1.731534 0.103652  
O 1.162460 -0.039909 -1.738643  
O -0.313099 -1.005454 2.487605  
O -2.400015 0.520671 1.541322  
O -1.355378 2.552905 0.321607  
O -1.422658 1.078371 -2.071559  
O -3.045336 -0.792704 -0.774101  
O 1.395785 2.282925 -0.087764  
O -1.244857 -3.015991 -0.723044  
H 3.704578 -0.154025 0.268056  
H -2.540675 -0.178861 -1.350653  
H -2.739550 -0.014635 0.782604

H -1.698670 -0.032135 1.959097  
H -2.525962 -1.619788 -0.776693  
H -0.402534 -2.527226 -0.378324  
H -0.525188 0.699515 -1.991518  
H -1.466615 1.742314 -1.358793  
H 0.421249 -0.420480 2.724185  
H 0.018657 -1.411806 1.650904  
H 1.395152 1.656427 -0.830568  
H 0.452040 2.456435 0.097283  
H 1.762875 -0.442381 1.075463  
H 1.993118 1.075581 1.152545  
H 3.170664 -0.132237 -1.141530  
H 1.027458 -0.777429 -1.006450  
H -1.814598 3.352304 0.591173  
H -1.752993 1.786409 0.856358  
H 1.583170 -2.348018 0.137614  
H 1.324165 -0.491056 -2.572512

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oh2.10h2o, E= -839.805321  
O 0.692691 -2.579071 0.461155  
O -1.496287 -0.835785 -2.056245  
O -0.586954 0.387220 1.737553  
O -2.241538 2.447852 0.705787  
O -1.833034 -1.534166 0.531997  
O -3.627221 0.273638 -0.216387  
O 1.333156 -1.211828 -1.717688  
O 0.343350 1.155096 -0.679986  
O 1.993793 -0.726277 2.098144  
O 3.428330 0.102176 -0.226613  
O 2.423368 2.840505 -0.614700  
H -1.196370 0.045982 -1.792579  
H -1.638545 -1.279453 -1.177875  
H 1.168367 -1.814521 -0.933715  
H 0.506183 -1.283100 -2.225993  
H 1.191671 -0.174964 2.134102  
H 2.543398 -0.366999 1.373679  
H 0.062787 0.873737 0.230765  
H 0.780113 0.352223 -1.050608  
H -1.120034 -0.407696 1.399662  
H -1.212260 1.133801 1.771199  
H -0.243898 -2.258276 0.524206  
H -2.310555 -2.252993 0.955259  
H -1.544815 2.508955 0.040975  
H -2.838971 1.743415 0.356505  
H 2.899574 -0.344956 -0.908376  
H 3.309869 1.050785 -0.399053  
H 1.571168 2.300609 -0.631161  
H -3.524807 0.142693 -1.166895  
H -3.019530 -0.434365 0.157229  
H 1.179413 -2.089750 1.158550

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oh2.10h2o, E= -839.804372  
O 0.356728 -0.110468 0.995580  
O 3.587934 -0.018410 -0.648508  
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O -2.045558 -1.098305 2.018532

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H 1.070379 -0.849413 0.888878  
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H 1.498769 -2.963691 -0.300146  
H -2.558694 1.517147 0.472635  
H -3.525550 0.551935 -0.142260  
H -2.155520 0.693586 -1.740269  
H -2.366069 -0.813045 -1.648935  
H 1.556834 3.098790 -0.068303  
H 0.757233 4.421658 0.077681  
H -0.338967 -0.414653 1.615093

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O 0.366681 -2.358891 -0.901842  
O -2.314881 1.685091 0.985907  
O 2.166959 -0.398852 -1.774072  
O 0.653330 1.833967 -1.814818  
O -2.045578 1.063055 -1.836077  
O 3.931379 -0.136388 0.165503  
O 1.867998 0.444092 2.136683  
O 0.448055 2.455790 0.883005  
O 0.229577 -1.788094 1.848982  
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H -2.704493 -2.050105 -1.511730  
H 3.274447 -0.229219 -0.611593  
H 1.630475 0.435225 -1.850274  
H -2.272851 1.473259 -0.987076  
H -2.036769 0.094274 -1.632232  
H -2.392488 0.713549 1.194632  
H -2.849524 2.153202 1.632213  
H 0.461541 -3.231641 -1.291763  
H 1.526481 -1.090621 -1.513076  
H -0.281383 1.573841 -1.960909  
H 0.408819 -2.089139 0.937023  
H -0.697074 -1.479898 1.804903  
H -3.121931 -1.428516 1.719252  
H -2.318892 -1.265928 0.264659  
H -0.484303 2.200392 0.990051  
H 0.667050 2.140047 -0.879385  
H 0.966046 1.772399 1.368957  
H 1.303265 -0.359282 2.091222  
H 2.625439 0.257239 1.553494

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oh2.10h2o, E= -839.803396  
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O 1.678503 -1.640040 -1.999726  
O -0.423697 -2.483922 -0.487536  
O -2.778961 -1.329148 -0.221748  
O -2.691787 1.321034 -1.371103  
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H 0.679525 -2.041072 2.813387  
H -0.013063 -2.376789 0.392913  
H 0.301733 -2.299180 -1.137557  
H 2.284289 2.107992 0.198556  
H 0.978320 3.355869 -0.674766  
H -2.935088 0.444807 -1.028466  
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  
H -1.954101 2.143771 0.223034  
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H 2.109244 -1.141217 1.011891  
H 1.257764 -0.779749 -2.188065  
H -3.449778 -2.011355 -0.311061  
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H 0.417232 1.367243 -1.127122  
H -0.209855 -0.061912 -0.904511

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oh2.10h2o, E= -839.802248  
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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  
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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  
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H 2.992099 -0.393530 -1.272387  
H -0.513830 1.632853 1.955742  
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H -1.727485 -1.802718 1.421900  
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oh2.10h2o, E= -839.801865  
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O -2.534481 -0.003429 1.901669  
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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  
H 0.630724 -1.937830 -1.249421  
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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  
H -0.687347 2.654564 -0.330570  
H -0.849142 1.821211 0.907397  
H 0.764738 -0.334381 -2.503685

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oh2.10h2o, E= -839.801419  
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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  
O 2.771098 -0.751764 -1.389492  
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H 0.297925 0.550282 -0.462826  
H -0.043810 1.787360 -1.340009  
H -0.939925 0.564869 1.168324  
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oh2.10h2o, E= -839.799932  
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O -0.277475 0.186081 1.277578  
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O 0.722605 1.797252 -0.653791  
O 3.357036 1.302191 -0.201153  
O -0.305662 -2.041435 -0.459959  
O 2.331344 -2.300720 0.121834  
O 2.382027 -0.262104 1.974248  
O 1.521965 -0.466215 -2.037605  
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H 0.402728 1.229140 0.093170  
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H 2.407842 -1.706081 -0.643021  
H -1.962397 2.658949 0.092231  
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oh2.10h2o, E= -839.799669  
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O 2.532420 0.971616 -0.740072  
O 0.328978 -0.406615 -1.442362  
O -1.031776 1.772378 -1.852195  
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oh2.10h2o, E= -839.799635  
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O -2.662589 1.973443 -0.372665  
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O -1.323458 -1.618508 1.976015  
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H 2.274058 2.061196 -0.340727  
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oh2.10h2o, E= -839.799503  
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oh2.10h2o, E= -839.799222  
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H -2.575531 -1.176212 0.279052  
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oh2.11h2o, E= -916.271768  
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O -0.458422 -2.033182 0.585543  
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H -2.763374 0.867447 -1.254177  
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H -3.141742 -0.891780 -0.229192  
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oh2.11h2o, E= -916.267860  
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O -3.245924 -1.138455 0.877546  
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H 1.339765 0.230378 1.916195  
H 0.548689 1.042989 0.831703

H -4.089685 -1.579075 1.007873  
H -3.218558 -0.824741 -0.080922  
H 2.092712 -0.043791 -2.734036

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oh2.11h2o, E= -916.267420  
O 1.222814 0.724790 2.484154  
O -1.233006 -0.435950 2.464503  
O -3.008058 1.083736 0.846934  
O 2.820030 -1.047380 0.918210  
O -1.088216 2.585267 -0.640643  
O 1.240371 2.527237 0.473875  
O 2.996253 0.957789 -1.021443  
O 1.171522 -0.637103 -2.506609  
O -1.170785 0.441163 -2.377854  
O 1.185878 -2.541429 -0.438933  
O -1.181642 -2.380391 0.553472  
O -2.729395 -1.101751 -0.845937  
H 0.320710 0.315071 2.532124  
H 3.507166 -1.618512 1.271390  
H 1.787802 0.049429 2.068392  
H -1.520773 -3.203326 0.916731  
H 0.240683 -2.510365 -0.048969  
H -1.782779 -0.163391 -1.880507  
H -1.147326 1.269158 -1.852349  
H -1.177842 -1.189740 1.823750  
H -1.885404 0.167884 2.056871  
H 0.238982 -0.201469 -2.493275  
H -2.386644 1.685441 0.398768  
H -3.070921 0.314358 0.243242  
H 3.099989 0.271902 -0.331328  
H 2.471800 0.515176 -1.712476  
H 1.209458 1.947847 1.281642  
H 1.894534 2.086849 -0.111557  
H -1.253315 3.504096 -0.868071  
H -0.175413 2.561185 -0.191711  
H -2.068388 -1.736727 -0.227871  
H -3.411030 -1.652752 -1.237999  
H 2.176294 -1.650378 0.419509  
H 1.126292 -2.169566 -1.334144

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oh2.11h2o, E= -916.267291  
O 2.775235 2.037951 -0.387834  
O 0.050959 1.862443 -0.589434  
O -0.214294 0.712126 1.864421  
O 2.607554 0.490891 1.981061  
O 2.612112 -1.950637 0.440254  
O 0.057036 -0.609973 -1.785130  
O 2.835694 -0.332877 -1.912725  
O -2.798874 1.868362 -0.653294  
O -2.608608 -0.709155 -1.893565  
O -2.475346 -1.689213 0.227506  
O -2.922775 0.314205 1.654019  
O 0.022667 -1.817221 0.773225  
H 2.826260 1.620410 0.496492  
H 2.923614 1.290524 -1.004946  
H -2.781253 0.167209 -1.477519  
H -3.032808 -1.997431 -0.495359  
H -0.944166 -1.970792 0.507845  
H -0.919332 -0.686136 -1.981883  
H 0.143951 -1.100199 -0.944600

H -1.857845 2.115360 -0.674120  
H -2.937367 1.490278 0.236658  
H -0.017181 -0.962783 1.259075  
H 1.624176 -2.062025 0.518992  
H -0.149698 1.211731 1.013054  
H -1.177252 0.636147 2.034586  
H 1.894233 -0.400490 -2.159980  
H 2.918259 -0.969648 -1.181381  
H 2.702116 -0.378759 1.554313  
H 1.658009 0.571533 2.182340  
H 0.995857 2.146277 -0.561970  
H 0.063609 1.028229 -1.115319  
H -3.633502 0.161639 2.281259  
H -2.836435 -0.541980 1.053684  
H 3.005887 -2.784311 0.710748

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oh2.11h2o, E= -916.267196  
O -0.493169 -0.259013 -1.815099  
O 1.773402 0.324132 -0.776946  
O 2.649647 2.778340 -1.188642  
O -1.514643 1.690508 -0.331636  
O 3.271803 -2.022541 -0.760761  
O -1.582143 -0.136383 1.624531  
O -0.494354 -2.189480 0.115810  
O 1.865904 -2.353640 1.512829  
O -2.944207 -1.409318 -1.414568  
O 0.595408 3.108347 0.831660  
O -4.087079 0.398099 0.392720  
H -1.124405 1.087559 -1.025191  
H -0.816491 2.315283 -0.041514  
H 0.858570 2.363842 1.402740  
H 1.317238 3.184289 0.182517  
H 2.862441 -2.663826 -1.350190  
H 2.875257 -2.214951 0.130287  
H 0.883758 0.093095 -1.241006  
H 2.368829 -0.447255 -0.889069  
H -0.368239 -1.637473 -0.693635  
H -0.954681 -1.565967 0.719751  
H -2.115639 -0.911848 -1.640297  
H -2.591798 -2.150159 -0.905020  
H -1.523693 0.567171 0.921718  
H -2.545414 -0.211178 1.721692  
H 1.835108 -1.469251 1.917958  
H 0.999438 -2.412936 1.042544  
H -3.507296 1.138385 0.155967  
H -3.828904 -0.283374 -0.264782  
H 2.374420 1.805596 -1.106719  
H -0.416939 -0.255474 -2.773492  
O 1.186592 0.456063 1.904458  
H 1.347007 0.369324 0.934361  
H 0.254137 0.218220 2.046528

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oh2.11h2o, E= -916.265162  
O -1.701001 2.472828 -0.555715  
O 0.796390 3.834824 0.067904  
O 1.689605 1.299320 -0.296107  
O -0.357405 0.181322 -1.305253  
O 0.610621 -2.386264 -0.951280  
O -1.804320 -3.045812 0.315904  
O -2.980952 -0.988686 -1.170262

O -3.443424 0.873996 0.915739  
O -1.017749 -0.532153 1.364329  
O 1.605737 0.157061 2.086675  
O 4.018254 -0.182589 -1.045152  
O 2.793024 -1.931605 0.517726  
H -1.236228 1.663699 -0.879316  
H -1.001765 3.003864 -0.139557  
H 0.770111 4.238291 -0.805291  
H 1.232949 2.961663 -0.074426  
H 0.889754 0.838636 -0.770783  
H 2.510537 0.948996 -0.691407  
H -2.102024 -0.588958 -1.323665  
H -3.375634 -0.391006 -0.502256  
H -2.721352 0.413460 1.377445  
H -2.967536 1.595429 0.452141  
H -0.172464 -0.331292 1.806046  
H -0.855496 -0.329115 0.423290  
H 3.611761 -0.915922 -0.464214  
H 1.669087 0.670709 1.229957  
H 1.821909 0.770487 2.794499  
H 0.285410 -1.474049 -1.140085  
H -0.168363 -2.827192 -0.550816  
H -2.369326 -2.507338 -0.279451  
H -1.553302 -2.382726 0.982583  
H 1.979281 -2.204732 0.008899  
H 2.457137 -1.397981 1.256873  
H -0.374694 0.227138 -2.266535

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oh2.11h2o, E= -916.264805  
O -0.536569 -0.335885 -1.829127  
O 1.677701 0.495507 -0.733987  
O 1.868552 3.135585 -1.146819  
O -1.697155 1.420765 -0.174295  
O -1.509432 -0.569280 1.642347  
O -0.128811 -2.357906 -0.000565  
O -2.914291 -1.458830 -1.693253  
O 2.226742 -2.231880 1.380486  
O 3.522279 -1.583615 -0.882738  
O 1.149223 0.413637 1.965174  
O 0.175671 3.014715 1.099072  
O -4.111419 -0.063312 0.513416  
H -1.252946 0.929729 -0.914837  
H -1.071497 2.086641 0.191067  
H 0.571923 2.288178 1.613795  
H 0.835756 3.218683 0.406887  
H 3.193363 -2.251757 -1.492540  
H 3.181537 -1.873416 0.006070  
H 0.837818 0.151353 -1.185230  
H 2.385010 -0.165008 -0.893962  
H -0.158889 -1.768607 -0.787221  
H -0.717958 -1.895041 0.629043  
H -1.974571 -1.054487 -1.727292  
H -1.556487 0.172479 0.984619  
H -2.449780 -0.735933 1.804828  
H 2.077876 -1.392075 1.848562  
H 1.371512 -2.376239 0.903901  
H -3.553428 0.710071 0.330691  
H -3.840274 -0.674805 -0.197064  
H 1.912599 2.147717 -1.065942  
H -0.403040 -0.283534 -2.780344  
H 1.305809 0.408580 0.990854

H 0.264563 0.029626 2.093057  
H 1.261165 3.291837 -1.876623

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oh2.11h2o, E= -916.263895  
O -0.068866 0.065250 1.120111  
O 1.887002 -0.518102 -2.056243  
O -1.412666 -1.859309 -0.315577  
O 1.040452 -2.957149 -0.981872  
O 1.676559 -1.640689 1.443304  
O 3.469914 -0.080316 0.316624  
O 1.804413 1.969902 1.424449  
O -0.177696 1.211942 -1.282257  
O -2.826014 -0.866322 2.035178  
O 0.830317 3.685999 -0.393811  
O -4.188525 0.974418 0.232942  
O -2.658735 0.111769 -1.754019  
H 1.146184 0.112065 -1.928293  
H 2.524166 -0.280510 -1.360907  
H 1.064860 1.300979 1.420724  
H 2.562316 1.469334 1.079655  
H -2.509964 -1.496941 1.368659  
H -3.386501 -0.252158 1.528403  
H -0.187341 0.833168 -0.357510  
H 0.127967 2.133950 -1.172721  
H -0.879124 -1.160539 0.135913  
H -0.718081 -2.454655 -0.671097  
H 0.865067 -0.918995 1.374503  
H 1.711928 -1.943691 2.354357  
H 1.330380 -2.176818 -1.504765  
H 1.317279 -2.719528 -0.077259  
H -3.642081 0.678225 -0.571986  
H -1.848417 0.664880 -1.780015  
H -2.309995 -0.736394 -1.396665  
H 1.277310 3.127917 0.298986  
H 0.113049 4.125402 0.073295  
H 4.369247 -0.416633 0.353039  
H 2.894172 -0.735734 0.806500  
H -0.831657 0.067531 1.716531

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oh2.11h2o, E= -916.263147  
O 2.186285 1.211148 2.155042  
O -0.293116 0.346139 1.383002  
O 0.399212 -2.141082 0.688843  
O 3.105720 -1.234826 1.028829  
O 2.924440 -0.045165 -1.558027  
O -0.660401 1.671088 -0.948911  
O 2.025953 2.361363 -0.380774  
O -3.046223 0.070722 1.743637  
O -3.437329 1.805169 -0.497327  
O -1.708073 -0.245792 -1.557420  
O -2.323731 -2.183723 0.091663  
O 0.723837 -1.386717 -1.944448  
H 2.613222 0.365138 1.911093  
H 2.259754 1.757831 1.343276  
H -3.437238 1.269503 0.321982  
H -2.460797 0.370974 -1.492690  
H -0.114880 -0.884989 -2.024491  
H -2.503770 2.075553 -0.590043  
H -0.467195 1.488431 -1.875186  
H -2.096081 0.278019 1.845500

H -3.017952 -0.800269 1.313485  
H 0.650495 -1.777163 -1.042472  
H 2.065054 -0.514119 -1.796365  
H 0.159171 -1.228484 1.007763  
H -0.473314 -2.564824 0.612516  
H 1.063862 2.229362 -0.513149  
H 2.428717 1.619845 -0.868696  
H 3.168555 -0.875634 0.124492  
H 2.301690 -1.780120 1.019971  
H 0.510248 0.736591 1.803586  
H -0.384782 0.774177 0.497211  
H -2.917723 -2.736768 -0.423752  
H -2.056377 -1.425510 -0.525521  
H 3.536752 -0.204139 -2.281376

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oh2.11h2o, E= -916.263089  
O 1.122897 -2.455253 0.759883  
O -1.136650 -2.451437 -0.350095  
O -3.006762 -0.961042 1.075647  
O 2.923103 -1.157306 -0.752365  
O -1.232043 0.766936 2.496031  
O 1.156889 -0.230435 2.459156  
O 2.864185 1.179675 0.921477  
O 1.264729 2.598998 -0.726588  
O -1.316629 2.630201 0.358636  
O 1.215360 0.466389 -2.481520  
O -1.166984 -0.732561 -2.284510  
O -2.725506 0.736013 -1.055208  
H 0.184483 -2.452546 0.302595  
H 1.253252 -3.335270 1.122978  
H 3.438325 -1.767970 -1.285762  
H 2.289404 -1.703486 -0.222149  
H -1.475129 -1.070006 -3.130265  
H 0.317099 0.031937 -2.447125  
H -1.830376 1.990380 -0.185677  
H -1.300800 2.240076 1.247643  
H -1.128065 -1.842481 -1.167930  
H -1.826731 -2.058402 0.229716  
H 0.363584 2.673052 -0.346713  
H -2.515912 -0.468154 1.755478  
H -3.069239 -0.328709 0.323510  
H 3.129024 0.473384 0.310913  
H 2.304447 1.785588 0.364526  
H 1.137675 -1.064218 1.948293  
H 1.801410 0.350697 1.971948  
H -0.277603 0.390245 2.525059  
H -2.068788 0.120888 -1.658573  
H -3.408175 1.092914 -1.628919  
H 1.791111 -0.106215 -1.950396  
H 1.190286 1.926872 -1.443492

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oh2.11h2o, E= -916.262929  
O -1.190563 0.305040 -2.412867  
O 1.021904 -0.810050 -2.317143  
O 1.067508 -2.465427 -0.369122  
O 2.753088 -1.101505 0.850152  
O -1.243917 -2.410732 0.978941  
O -3.010155 -1.047744 -0.912782  
O 2.946079 0.794432 -1.145155  
O -1.190611 -0.185725 2.623517

O -2.786950 1.156195 0.919369  
O -1.213125 2.528273 -0.768328  
O 1.238840 2.633079 0.164174  
O 1.402727 0.803330 2.342666  
H -0.230140 -0.178834 -2.430911  
H -3.695039 -1.455501 -1.449479  
H -2.372116 -0.628120 -1.541487  
H 1.322969 -3.361574 -0.605456  
H -0.374097 -2.464273 0.491753  
H 1.892219 0.080357 1.894787  
H 1.334250 1.498920 1.664688  
H 1.019453 -1.534670 -1.583268  
H 1.741558 -0.190587 -2.051920  
H -0.274211 0.166421 2.594894  
H 2.419118 1.510457 -0.743628  
H 3.056513 0.140849 -0.421127  
H -3.084378 0.406234 0.378796  
H -2.213553 0.735620 1.617452  
H -1.241355 1.963131 -1.561362  
H -1.816450 2.079367 -0.112405  
H 1.426354 3.565305 0.302789  
H 0.300455 2.586395 -0.192194  
H 2.057824 -1.750070 0.367404  
H 3.407706 -1.646846 1.293041  
H -1.877480 -2.075328 0.326168  
H -1.158194 -1.040575 2.134096

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oh2.11h2o, E= -916.262650  
O 0.029125 -2.595427 -1.032332  
O -2.682078 -2.109973 -0.168875  
O -2.272629 0.106165 -1.328415  
O 0.361781 0.055771 -1.561968  
O 1.094097 2.651251 -0.869530  
O 3.048086 1.508097 0.801331  
O -0.586464 2.653858 1.257916  
O 3.048371 -0.572456 -0.986197  
O 2.060703 -2.511618 0.822650  
O 0.489891 0.010019 1.234651  
O -1.540684 -1.732252 2.199129  
O -2.937712 2.425588 0.017178  
H 0.147225 -1.649931 -1.311452  
H -0.909109 -2.671242 -0.800981  
H -3.540941 -2.476591 -0.393061  
H -2.590543 -1.199308 -0.642397  
H -1.274728 0.158490 -1.451590  
H -2.552193 0.922636 -0.858211  
H 2.125892 -0.362517 -1.255026  
H 2.942485 -1.369683 -0.431442  
H 1.732366 -1.728892 1.289233  
H 1.323027 -2.720714 0.206402  
H -0.214249 -0.585122 1.558250  
H 0.449195 -0.004230 0.256029  
H -2.907100 3.151953 -0.613122  
H -2.106058 2.530977 0.559874  
H -2.046834 -1.944921 1.357065  
H 0.806073 1.762751 -1.190397  
H 1.909008 2.450366 -0.364671  
H 3.231768 0.772682 0.170207  
H 2.338154 1.144781 1.348755  
H 0.004366 2.841800 0.485469  
H -0.288162 1.759614 1.506785



H 0.520472 0.104906 -2.510032  
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oh2.11h2o, E= -916.262558  
O 0.435569 1.456070 2.402980  
O -0.090951 3.013268 0.051299  
O 1.914492 2.561009 -1.623372  
O 2.756771 0.294988 -1.133057  
O 1.451470 -1.810742 -1.642225  
O -2.614745 1.748201 -0.043478  
O -1.919921 0.145807 2.085021  
O -1.445835 -2.231202 1.216620  
O -1.298916 -1.990950 -1.545758  
O -2.843898 0.067124 -2.252549  
O 1.324906 -2.750139 1.003682  
O 2.431049 -0.200236 1.552276  
H 1.183019 0.856509 2.153184  
H -0.116071 3.972189 0.116342  
H 0.332422 2.057841 1.644758  
H 3.695867 0.207443 -1.323632  
H 2.292365 1.549811 -1.448596  
H -0.331360 -1.863718 -1.654718  
H -1.422883 -2.139186 -0.586035  
H 2.588821 0.033825 0.605649  
H 2.096632 -1.118888 1.514961  
H -2.222577 -0.679267 -2.027951  
H -3.715607 -0.338448 -2.268362  
H 0.372951 -2.616738 1.171296  
H 1.425277 -2.576027 0.047786  
H -1.758316 2.210742 -0.113956  
H -2.695254 1.206045 -0.856401  
H -1.062242 0.587072 2.317578  
H -2.280020 0.699208 1.351777  
H -2.014865 -2.822851 1.715793  
H -1.626313 -1.290755 1.568035  
H 1.983972 -0.932441 -1.472419  
H 1.846551 -2.232713 -2.409479  
H 0.627710 2.804758 -0.617117

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oh2.11h2o, E= -916.262295  
O 2.487912 -0.665457 -1.960338  
O 3.094520 1.674918 -0.323059  
O 0.448288 1.637028 -0.157915  
O -0.213691 -0.167858 -1.771382  
O 3.554654 -1.003065 0.598127  
O -0.487687 -0.024147 1.811238  
O 1.458496 -1.925333 2.168681  
O -0.534054 -2.106947 0.034960  
O -3.236201 -2.572958 -0.560649  
O -2.854093 0.030358 -0.982797  
O -2.720019 1.606256 1.341954  
O -1.163623 3.732132 0.056520  
H 1.503586 -0.580353 -1.890359  
H 2.811783 0.227349 -1.768757  
H 3.408132 2.582969 -0.311885  
H 2.101203 1.719017 -0.223392  
H 0.177332 0.981209 -0.925728  
H 0.202773 1.119531 0.645777  
H -0.372042 -1.530447 -0.757970  
H -1.426765 -2.480763 -0.100721  
H -3.215241 -1.582278 -0.680347

H -3.365117 -2.921730 -1.447614  
H -2.907938 0.606456 -0.191580  
H -1.902802 0.020688 -1.255478  
H -0.514173 2.969377 -0.102637  
H -2.305124 2.430160 1.034927  
H -1.997399 1.093296 1.748988  
H -0.717629 -0.737022 1.166872  
H 0.250485 -0.461620 2.285503  
H 0.892809 -2.281445 1.462291  
H 2.264938 -1.620823 1.696696  
H 3.206279 -1.188807 -0.299131  
H 3.589075 -0.032713 0.585910  
H -0.360194 -0.051466 -2.714085

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oh2.11h2o, E= -916.261426  
O -1.851551 2.341606 -0.604271  
O -0.398747 0.051229 -1.370891  
O 1.601990 1.403060 -0.164327  
O 1.580365 -0.261426 2.113323  
O 0.403700 3.757177 0.340834  
O 0.623527 -2.279180 -0.961147  
O 3.168818 -1.883739 0.349006  
O 4.194456 0.394996 -1.086998  
O -3.537180 0.764791 0.876040  
O -1.803938 -2.972053 0.339707  
O -2.995451 -1.062898 -1.205286  
O -0.932857 -0.578496 1.316904  
H -1.334134 1.571581 -0.923648  
H -1.189260 2.942237 -0.211215  
H 0.737197 4.366908 -0.324048  
H 0.922683 2.922412 0.204653  
H 0.903820 0.892304 -0.661177  
H 3.379547 0.896725 -0.928207  
H -2.126145 -0.646882 -1.392296  
H -3.402126 -0.457100 -0.551248  
H -2.835761 0.345097 1.396806  
H -3.056187 1.485378 0.409203  
H 0.617035 -0.439913 1.932875  
H -0.865154 -0.188328 0.424973  
H 4.008961 -0.453949 -0.646169  
H 1.750405 0.895094 0.655755  
H 1.635335 0.125774 2.991151  
H 0.233474 -1.337609 -1.186322  
H -1.012702 -3.129206 -0.202472  
H -2.388681 -2.442803 -0.256089  
H -1.239816 -1.503174 1.141371  
H 2.407122 -2.125727 -0.206605  
H 2.766439 -1.405018 1.092128  
H -0.337117 0.285657 -2.302561

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oh.6h2o, E= -534.645268  
O -2.227794 0.492702 -0.835302  
O 0.356242 -0.366316 -1.595157  
O -1.161192 -2.072016 -0.152103  
O 0.238167 -0.868585 1.965082  
O 1.142853 1.992851 -0.595415  
O 2.312606 -0.704968 0.028497  
O -0.873156 1.664677 1.371766  
H -1.367265 0.292832 -1.263642  
H -1.952998 0.976318 -0.030198

H -0.177121 1.949441 0.745750  
H -0.533052 0.810783 1.713736  
H 1.054765 -0.750232 1.441578  
H -0.325058 -1.393866 1.355701  
H -1.904016 -1.445282 -0.199031  
H -0.527955 -1.613511 -0.765728  
H 1.916283 1.605884 -0.167385  
H 0.777089 1.209395 -1.095022  
H 2.642860 -1.606595 -0.014305  
H 1.577829 -0.640401 -0.687713  
H 0.516827 -0.501511 -2.532687

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oh.6h2o, E= -534.642390  
O 0.853640 0.122690 1.462716  
O 1.875842 1.501430 -0.675858  
O -1.500545 1.352820 1.121525  
O -2.903967 -0.990088 -0.175332  
O -0.199736 -1.554159 -0.141735  
O -0.879817 0.839333 -1.547225  
O 2.729031 -1.210532 -0.156203  
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  
H 0.153395 -0.958306 0.613166  
H 0.617828 -1.923209 -0.503326  
H -2.746979 -0.342454 -0.876316  
H -2.038680 -1.443230 -0.128921  
H -0.563749 -0.035698 -1.245142  
H -1.123822 1.264517 -0.696207  
H 1.028594 0.025808 2.401728

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oh.6h2o, E= -534.642290  
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O 1.500532 -1.173988 0.995951  
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O 3.148855 0.697759 -0.036456  
O -2.576251 1.394730 -0.210402  
O 0.417592 1.489765 -0.593891  
O -2.057711 -1.521426 -0.077525  
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  
H -2.009427 1.040678 0.523709  
H -0.840589 0.498179 2.356023  
H 0.317519 -0.223752 -1.410494  
H 1.378638 1.500210 -0.447215  
H 1.208891 -1.466038 0.110230  
H 0.691009 -0.673111 1.306429  
H 2.620432 0.018030 0.466059  
H 3.290645 0.276099 -0.890449  
H 0.043020 1.133142 0.261671

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oh.6h2o, E= -534.642096  
O 2.317781 -0.732953 -0.397308  
O 0.688537 -0.904176 1.952873

O -0.398052 1.703435 1.351705  
O 1.025263 1.756923 -0.854803  
O -0.129516 -0.393439 -1.711153  
O -1.078390 -2.057231 0.143037  
O -2.387985 0.492379 -0.415543  
H 1.522714 -0.793573 -0.976404  
H 1.937385 -0.851881 0.495130  
H 0.050180 -1.425615 1.413903  
H 0.332461 0.000268 1.914140  
H -0.356849 2.550441 1.803194  
H 0.164424 1.800122 0.519600  
H 1.815647 1.239535 -0.616570  
H 0.501686 1.027455 -1.335511  
H -1.852278 -1.482925 0.253711  
H -0.640919 -1.600029 -0.631162  
H -1.924752 0.984649 0.280355  
H -1.650580 0.232079 -1.024492  
H -0.200218 -0.600026 -2.646356

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oh.6h2o, E= -534.641771  
O -0.112225 -0.100849 2.046432  
O 1.146487 -1.794865 0.227531  
O 2.490827 0.096000 -0.622996  
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  
O 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  
H -0.371550 1.671259 -0.796348  
H 1.498577 2.608846 0.570944  
H 1.710711 1.099099 -0.079198  
H 1.783820 -1.007573 -0.163850  
H 2.411626 0.134270 -1.581973  
H -1.759858 -1.205911 -0.621944  
H -0.312308 -1.693485 -0.832114  
H 0.321407 -0.830279 1.556277  
H 1.694686 -2.566907 0.386190

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oh.6h2o, E= -534.641114  
O -0.306527 -0.279918 2.018657  
O 0.991054 -1.812175 0.283610  
O -0.958284 -1.291787 -1.431607  
O -2.633179 0.087039 0.530103  
O -0.900214 1.517069 -1.382372  
O 2.429040 -0.042360 -0.656969  
O 1.134553 1.822726 0.630526  
H 0.153352 0.544724 1.795160  
H -1.885911 -0.068550 1.153183  
H -2.286191 0.774423 -0.063832  
H -0.791044 0.554587 -1.547584  
H -0.237163 1.732420 -0.703696  
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  
H -0.221389 -1.599539 -0.827399

H 0.176167 -0.957942 1.461429  
H 1.334280 -2.689329 0.467371  
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oh.6h2o, E= -534.641072  
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H -2.640010 -1.003560 -0.091598  
O -3.324863 -0.326386 0.026199  
H -2.796753 0.488567 0.085352  
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H 1.100745 2.480376 0.056730  
H -0.670254 1.108931 0.680930  
O -1.202337 1.676651 0.059629  
H -0.901509 1.384845 -0.812228  
H 0.176375 -0.467861 -1.356510  
O 0.732564 0.135243 -1.885739  
H 1.204511 0.703705 -1.245109  
H 1.682947 -1.130559 0.801783  
O 2.176854 -1.761513 0.224237  
H 2.161694 -1.317778 -0.633680  
H -0.396753 -1.022158 0.594505  
O -0.752571 -1.624315 -0.135121  
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oh.6h2o, E= -534.640928  
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O -1.310234 1.360994 0.761358  
O 0.468469 1.869076 -1.021762  
O 2.764947 0.023096 0.306061  
O 1.068183 -0.762344 -1.631313  
O -2.734629 -0.308755 -0.555435  
O -0.644683 -2.054051 0.102630  
H -0.299418 -1.556270 0.878839  
H 1.186833 -0.038324 1.538963  
H 3.250364 -0.730890 0.653384  
H 2.226634 -0.341109 -0.449588  
H 0.704327 0.152259 -1.604748  
H 0.435199 -1.305846 -1.102074  
H -1.480162 -1.585291 -0.113553  
H -2.248660 0.399390 0.011046  
H -2.499795 -0.074054 -1.458812  
H 1.285860 1.883464 -0.510334  
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H -0.306711 0.410006 1.636134  
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oh.6h2o, E= -534.639497  
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O -2.699858 -0.023390 -0.551075  
O -1.079871 1.761467 0.009783  
O 1.425158 1.503748 -1.161814  
O 1.384030 -1.363185 -1.327352  
O 2.485583 -0.103723 0.997096  
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H 1.634181 -0.051759 1.482189  
H 2.290786 -0.741244 0.282860  
H 1.334534 -0.416516 -1.560300

H 0.510441 -1.557964 -0.924346  
H -1.420528 -2.653254 -0.047845  
H -1.799617 -1.064906 -0.277131  
H -1.830163 1.030218 -0.274751  
H -3.384953 -0.032242 0.125950  
H 1.926381 1.214148 -0.377000  
H 0.514958 1.645008 -0.821053  
H -0.471797 0.760626 1.442712  
H -1.491730 2.628709 -0.007971

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oh.6h2o, E= -534.638951  
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O 0.375671 -2.143528 -0.626910  
O -4.144580 0.441547 -0.136649  
O 0.427688 1.471559 -0.868977  
O -1.458851 -0.021273 0.067298  
O 0.495222 -0.971577 1.985076  
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H 1.077796 -0.215572 1.761301  
H 0.584414 -1.571500 1.219508  
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H 1.538367 0.444856 -1.459771  
H 2.779457 -0.087409 -0.743228  
H 0.260830 2.296231 -1.330033  
H -0.802843 0.636014 -0.350123  
H -1.051556 -0.245141 0.923563  
H -3.170806 0.366953 0.009108  
H -4.333263 -0.318024 -0.695495  
H 1.806023 1.980588 1.781120

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oh.6h2o, E= -534.638741  
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O 0.182425 -0.173028 1.943176  
H 0.447081 -0.852148 1.252358  
H 0.500230 0.660709 1.566922  
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H 3.325556 -0.325321 0.206535  
H 1.965274 -0.936955 -0.413939  
O 1.212499 1.844474 0.057617  
H 1.832387 1.106989 -0.239259  
H 1.655789 2.672928 -0.141773  
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H -1.913873 1.244445 -0.252188  
H -0.519051 1.738925 -0.674696  
O -2.454758 -0.133394 0.982784  
H -1.604957 -0.151593 1.474363  
H -2.282111 -0.735014 0.229263  
O -1.436695 -1.276415 -1.397645  
H -0.559579 -1.493580 -0.972728  
H -1.370182 -0.331599 -1.612085

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oh.6h2o, E= -534.638335  
O 1.171751 -1.739033 -0.071925  
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O -1.636959 1.687183 -1.048895  
O -1.452702 -1.392022 -1.242665

O -2.120533 -0.262516 1.047988  
O 0.785909 1.854707 0.216104  
O 0.320252 -0.166633 1.812785  
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H 0.367723 -1.752357 -0.618231  
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H -2.200961 0.604774 0.615273  
H -1.185313 -0.236994 1.474245  
H 0.560798 -0.207244 2.740662  
H 0.635209 1.150807 0.924581  
H 1.462346 1.454930 -0.354655  
H -0.750483 1.838970 -0.633736  
H -1.552233 0.818625 -1.465762  
H 2.298571 -0.607837 -0.667361  
H 3.282141 0.331020 0.040353

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oh.6h2o, E= -534.636459  
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H -2.134103 -2.043519 -0.171301  
O -3.530360 0.868449 0.008014  
H -3.039499 0.003635 0.132411  
H -3.036035 1.471773 0.572047  
O -0.728735 0.447220 -1.237986  
H -1.195963 -0.318406 -0.672747  
H -1.477885 0.968993 -1.545255  
O 0.504290 -1.229156 1.391377  
H -0.442861 -1.332685 1.069750  
H 0.593404 -0.262813 1.481197  
O 0.746006 1.607771 0.813839  
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H 0.192628 1.303993 0.058978  
O 1.589465 -1.090218 -1.140261  
H 0.863047 -0.553182 -1.507881  
H 1.236903 -1.321393 -0.245003  
O 3.359382 0.651485 -0.054571  
H 3.479840 0.192127 0.783294  
H 2.798945 0.021501 -0.578756

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oh.6h2o, E= -534.636263  
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O -3.015555 -1.097811 -0.516252  
O -2.220371 1.188864 0.653176  
O -0.048712 1.340276 -0.711656  
O 2.770637 1.073663 -0.850090  
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H -3.147140 -0.797612 -1.421008  
H -2.801677 -0.261063 -0.017357  
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H -1.805996 1.003006 1.505303  
H 1.801120 1.214863 -0.787803  
H 2.876530 0.151167 -0.570434  
H 2.150100 -0.975809 1.153175  
H 1.558492 -1.684416 -0.043938  
H 0.071059 -0.487051 1.236513  
H 0.520335 0.926050 1.069154  
H -0.053483 1.946783 -1.456258

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oh.6h2o, E= -534.635054  
O -0.155977 -1.118685 -0.424236  
H 0.601030 -1.346165 -0.976897  
O 0.584173 0.983184 0.878531  
H 0.499008 0.832173 1.824513  
H 0.134871 -0.300526 0.117944  
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H 2.012836 1.042532 0.367816  
O 2.829375 -1.736414 -0.451729  
H 2.971003 -0.764221 -0.357388  
H 2.180118 -1.935763 0.231776  
O -2.611850 0.216006 -0.990806  
H -1.779187 -0.288449 -1.042260  
H -2.320634 1.070985 -0.613264  
O -1.309969 2.533952 -0.012034  
H -0.566121 1.969235 0.388795  
H -0.921966 2.890932 -0.816660  
O -2.527587 -2.003368 0.930600  
H -1.620611 -1.981289 0.582933  
H -2.919089 -1.247438 0.463134

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oh.7h2o, E= -611.109645  
O 0.000082 1.025976 -1.474615  
H 0.000151 1.544091 -2.284142  
O -2.455071 1.139845 -0.329680  
H -1.622141 1.101597 -0.873538  
H -2.137335 1.582593 0.470109  
O -0.000707 -1.494530 -1.563399  
H -0.000408 -0.451029 -1.615312  
H -0.000463 -1.823862 -2.465418  
O 2.455501 1.138340 -0.330141  
H 1.622348 1.100637 -0.873730  
H 2.138473 1.581451 0.469723  
O 0.001537 1.936029 1.222355  
H 0.000415 1.766980 0.259731  
H 0.000662 1.033223 1.616918  
O 2.057740 -1.554554 0.348142  
H 2.379568 -0.650908 0.145052  
H 1.409519 -1.717081 -0.364433  
O -0.000131 -0.706970 2.091937  
H 0.772847 -1.074705 1.614138  
H -0.773511 -1.073915 1.614149  
O -2.058826 -1.553298 0.348583  
H -2.380159 -0.649467 0.145516  
H -1.410962 -1.716302 -0.364204

23

oh.7h2o, E= -611.108553  
O -2.066514 1.564554 0.086953  
O -2.479276 -1.209930 -0.068918  
O -0.105899 0.973994 2.026852  
O 0.283521 -1.754995 1.327609  
O -0.110981 -1.290442 -1.292102  
O 2.582077 -1.013911 -0.275832  
O 1.929888 1.679243 0.241561  
O 0.006817 1.186659 -1.771095  
H -0.026433 0.152135 -1.666462  
H 0.012740 1.377168 -2.712180

H -1.405832 1.598478 -0.632533  
H -2.398536 0.644096 0.039707  
H -1.659036 -1.278507 -0.639815  
H -2.162240 -1.505091 0.792902  
H -0.848350 1.269113 1.458363  
H -0.041985 0.009335 1.871075  
H 0.083436 -1.704401 0.356796  
H 1.250903 -1.680456 1.300359  
H 1.748408 -1.145370 -0.770069  
H 2.545940 -0.060854 -0.050321  
H 1.301464 1.525917 0.981395  
H 1.348059 1.668120 -0.541599  
H -0.065592 -1.951061 -1.987842

23

oh.7h2o, E= -611.107008  
O 0.715186 -0.471717 -1.552785  
H 0.937156 -0.688518 -2.462477  
O 2.679175 0.829546 -0.254491  
H 1.987104 0.440495 -0.857567  
H 2.891861 0.069642 0.303867  
O 1.727448 -1.914409 0.617833  
H 1.451617 -1.503834 -0.232854  
H 1.169514 -1.465063 1.274372  
O -1.210799 -1.791472 -0.552259  
H -0.461833 -1.286296 -1.053731  
H -0.770061 -2.551706 -0.158082  
O -0.977573 1.646500 -1.249585  
H -0.372952 0.890718 -1.469891  
H -1.782358 1.234375 -0.890533  
O 0.526034 2.085357 1.037406  
H -0.041681 2.127553 0.234995  
H 1.390575 1.792109 0.680952  
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H -0.103604 0.549184 1.650871  
H -0.743470 -0.728493 1.025207  
O -3.038375 0.145364 0.205189  
H -2.591576 -0.670006 -0.100257  
H -2.614405 0.308950 1.058657

23

oh.7h2o, E= -611.106674  
O 2.083700 1.637560 0.013439  
O 0.097990 1.075604 1.920418  
O -1.933614 1.636008 0.004901  
O -0.061189 1.133251 -1.724481  
O 2.522411 -1.125802 -0.214145  
O -0.135894 -1.685778 1.440925  
O -2.529636 -1.176097 -0.172404  
O 0.069475 -1.433587 -1.191538  
H 2.422894 0.724543 -0.095228  
H 1.463110 1.550879 0.769164  
H 0.081493 0.097105 1.832518  
H -0.675020 1.368406 1.404441  
H -2.383607 2.455133 -0.217210  
H -1.235038 1.488278 -0.718297  
H 0.751334 1.432901 -1.261220  
H -0.014908 0.128953 -1.658972  
H -1.104790 -1.694140 1.460235  
H 0.015610 -1.711218 0.453075  
H -2.568867 -0.211641 -0.064996  
H -1.682655 -1.308092 -0.659658

H 1.650542 -1.260140 -0.696407  
H 0.061173 -2.136420 -1.846194  
H 2.312787 -1.413823 0.681837

23

oh.7h2o, E= -611.106661  
O -0.127962 -1.366119 -1.627815  
H -0.364234 -1.884372 -2.400638  
O -1.899664 -1.263374 0.065378  
H -0.961993 -1.397928 -0.918458  
H -2.573205 -1.946848 0.099911  
O 0.138803 1.363222 -1.612819  
H 0.043483 0.394362 -1.760324  
H 0.034647 1.449417 -0.648854  
O 2.089290 -1.538295 0.047487  
H 1.386551 -1.565622 -0.635250  
H 2.384766 -0.607960 0.056849  
O 0.007578 -1.151924 1.951695  
H -0.757927 -1.304375 1.333966  
H 0.790455 -1.424990 1.433317  
O -0.028438 1.509234 1.344429  
H 0.015698 0.577111 1.679807  
H -0.969549 1.616684 1.093485  
O 2.526491 1.312926 0.012726  
H 2.076462 1.417433 -0.841931  
H 1.805120 1.525389 0.633296  
O -2.508611 1.298609 0.023183  
H -2.386121 0.299604 0.061120  
H -2.104049 1.537853 -0.820399

23

oh.7h2o, E= -611.105635  
O 0.340913 -0.387719 -1.569448  
O 2.266717 1.305269 -0.820316  
O 2.145532 -1.718975 -0.216277  
O -1.399122 1.474330 -0.676548  
O 0.517898 2.066800 1.268405  
O 0.658920 -0.644159 2.006949  
O -3.408446 -0.099053 0.047042  
O -1.121948 -1.808509 0.208486  
H -3.834062 -0.253864 -0.801499  
H -2.694445 0.573301 -0.159705  
H -0.656462 -1.330908 -0.528030  
H -1.995691 -1.378711 0.256072  
H 1.468069 -1.263969 -0.813729  
H 1.707964 -2.535125 0.047701  
H -0.779694 0.817138 -1.095024  
H -0.863652 1.834616 0.063370  
H 1.211528 1.983405 0.582845  
H 0.509730 1.173493 1.674294  
H -0.100392 -1.053251 1.534285  
H 1.393860 -0.873677 1.411039  
H 1.524162 0.768930 -1.221192  
H 2.822334 0.620885 -0.429177  
H 0.283045 -0.586126 -2.507597

23

oh.7h2o, E= -611.104970  
O -0.018090 0.008377 -1.559780  
O 1.208951 -1.752999 -0.037708  
O 1.277911 1.762991 -0.215924  
O -2.384101 1.098811 -0.903439

O 3.535281 -0.027744 0.053069  
O -0.999244 1.725302 1.462687  
O -0.723052 -1.013197 1.955877  
O -1.898096 -1.831920 -0.489454  
H -1.271780 -1.283085 -1.003987  
H -1.650031 -1.627990 0.435955  
H -2.789677 0.246207 -0.689656  
H -1.507633 0.803805 -1.272144  
H 0.784565 1.091600 -0.819323  
H 1.357565 2.571462 -0.729873  
H -1.613017 1.619765 0.704939  
H -0.133667 1.849220 1.026500  
H -0.843603 -0.038655 1.917102  
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  
H -0.461775 -0.453923 1.512871  
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  
H 0.438241 1.251399 -0.926926  
H -0.438448 -1.251635 -0.926752  
H 0.363587 -2.349780 -0.216093  
H 1.563813 -0.818370 -1.317245  
H 2.622617 -0.721167 -0.207322  
H 0.078664 0.761691 1.144491  
H -0.078519 -0.761664 1.144628  
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  
O -2.490826 -1.186185 -0.504902  
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  
O 1.095328 -0.529174 -1.387017  
O 2.653951 -1.566024 0.616722  
O -0.412356 -1.765805 0.376496  
O -1.105181 0.996972 -1.701304  
O -2.829907 -0.945370 -0.355788  
O 2.301063 1.384553 0.010318  
O -1.346575 0.306300 2.024064  
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  
H 2.633947 0.741824 0.651636  
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  
H -0.476014 -1.082073 1.075662  
H -2.162137 0.158829 1.527570  
H -0.939518 1.103717 1.596098  
H 0.696646 2.125694 0.496827  
H -0.627669 2.029146 -0.276857  
H 1.340229 -0.893895 -2.241101

23  
oh.7h2o, E= -611.101312  
O -0.314619 0.918772 -1.009216  
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  
O 2.557145 1.736099 -0.617508  
H 0.470684 -0.673661 -1.258980  
H 0.176197 -2.028518 -0.599531  
H -1.840115 -1.627476 0.219177  
H -0.724533 -1.459386 1.243001  
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  
H -1.337585 1.850933 0.161651  
H -2.692629 1.399813 0.652263  
H -0.139005 1.452095 -1.789106

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  
H -2.510264 0.641690 0.081689  
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 -1.164501 1.055284 1.783285  
H -1.560231 -0.444601 1.764981  
H 1.725436 -1.477590 -0.124871  
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  
O -0.005984 1.642446 -0.692828  
O 2.044594 1.446012 0.738352  
O 0.697762 -0.767668 -1.462397  
O 3.520977 -0.405537 -0.715541  
O -1.905990 1.473853 1.260942  
O -1.416420 -1.217923 1.864971  
O -1.843671 -1.920300 -0.814948  
O -2.665947 0.710611 -1.389549  
O 1.364591 -1.221948 1.226882  
H -1.750540 1.042908 -1.316820  
H -2.551548 -0.256527 -1.279845  
H -2.587073 1.269913 0.596820  
H -1.140482 1.660232 0.663529  
H 1.022144 -1.244466 0.308141  
H 1.602562 -0.277902 1.321057  
H 1.187472 1.605555 0.147909  
H 2.104631 2.172423 1.363525  
H -1.592097 -0.254952 1.773623  
H -0.444228 -1.291105 1.866103  
H -1.760525 -1.778089 0.154457  
H -0.951665 -1.747491 -1.160010  
H 3.197024 0.410691 -0.284357  
H 0.403007 0.177719 -1.279827  
H 1.653306 -0.708989 -1.620467  
H 0.039273 2.384164 -1.303056  
H 3.249444 -1.080463 -0.077854

26

oh.8h2o, E= -687.567154  
O 0.213193 -1.850295 -0.301590  
O -2.589934 -2.150873 -0.030839  
O -2.387857 0.349797 -0.968186  
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  
O -1.822261 2.019660 1.295050  
O 0.658088 2.226835 -0.077393  
H 0.214393 -1.104414 -0.984799  
H -0.700036 -2.192609 -0.279535  
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  
H 1.888186 -1.923616 0.533753  
H 0.112639 -0.647402 1.080916  
H 0.530585 0.825799 1.176775  
H -1.057117 2.438504 0.862656

H -1.395226 1.267859 1.741357  
H 0.397839 1.593022 -0.821653  
H 1.625265 2.172873 -0.114667  
H 0.214095 0.353942 -2.705115

26

oh.8h2o, E= -687.566997  
O 1.610515 2.288916 0.264713  
O 1.513071 0.531401 -1.870043  
O -1.157680 0.055505 -1.597369  
O -0.347584 -2.242469 -0.527971  
O -1.127647 -0.883550 1.718342  
O 1.557413 0.043898 1.850363  
O 2.387156 -1.546040 -0.091596  
O -3.296780 -0.094327 0.064292  
O -1.134856 1.889318 0.306676  
H 0.604535 -0.150138 1.946235  
H 1.616938 0.917059 1.388289  
H -1.053062 1.202137 0.984506  
H -1.135150 1.334064 -0.530047  
H -0.654830 -1.453625 -1.059891  
H 0.621380 -2.187139 -0.513519  
H 1.930988 -0.238505 -1.451806  
H 0.534237 0.354273 -1.812323  
H 1.711636 1.768485 -0.566312  
H 0.640081 2.420745 0.298460  
H -0.812220 -1.490377 1.002738  
H -2.020895 -0.654711 1.393872  
H 2.120303 -0.983035 0.694519  
H 3.196505 -2.000996 0.153451  
H -2.583539 -0.175493 -0.629859  
H -1.486881 0.145413 -2.495785  
H -3.258892 0.850625 0.258223

26

oh.8h2o, E= -687.565918  
O -1.074742 -0.165361 -1.702619  
O 0.899910 -1.955117 -1.300830  
O 2.691177 0.053256 -0.657964  
O 0.718610 1.823453 -1.451532  
O 0.047495 2.223721 1.349338  
O 1.556947 0.108482 1.818238  
O -0.059800 -2.153450 1.454578  
O -2.241169 -1.365506 0.283267  
O -2.420022 1.460634 0.126034  
H 0.468391 2.161711 -0.576810  
H 0.049024 1.103111 -1.629612  
H -1.674972 1.821449 0.635172  
H -1.986238 1.036742 -0.651928  
H 1.012353 -0.703000 1.805857  
H 2.083226 0.070237 0.976725  
H 2.213225 -0.749882 -0.967621  
H 0.669724 -2.234354 -0.400869  
H 0.173463 -1.310779 -1.540262  
H -1.463510 -0.226748 -2.579444  
H 0.593676 1.412058 1.575779  
H 0.369470 2.931904 1.912539  
H 2.128055 0.776484 -1.020047  
H -0.947804 -1.853625 1.071363  
H -0.238718 -2.920750 2.003716  
H -1.831318 -1.041427 -0.589094  
H -2.565302 -0.514029 0.626444



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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  
H -2.371131 0.921291 -1.106931  
H -1.965495 1.376714 0.264548  
H -1.040082 -0.289317 1.655850  
H -1.998081 0.608556 2.558537  
H 1.038846 2.010498 -0.092694  
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H 0.882544 -0.785508 -1.802897  
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H -0.042716 -1.615773 0.133524  
H 0.402924 -1.653665 2.213474  
H -2.070902 -1.443480 -0.883501  
H 0.033194 -2.811578 -0.914844

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oh.8h2o, E= -687.565057  
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O 0.435360 -0.183471 1.759802  
O 0.583054 -1.444099 -1.396667  
O -2.417801 -0.599111 -1.676214  
O 2.762710 -1.260332 0.496680  
O -2.286649 0.663694 1.893804  
O 0.747572 1.174468 -0.603001  
O -2.016848 1.967974 -0.633702  
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H -2.125673 -1.034233 -0.819891  
H -1.662805 -0.754412 -2.255751  
H -0.187285 -0.856494 1.309302  
H -0.214270 0.351624 2.245121  
H -0.116826 -1.639473 -0.710505  
H 1.421838 -1.593538 -0.921026  
H -2.159079 -0.208746 1.464120  
H -2.288697 1.273075 1.128852  
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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  
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oh.8h2o, E= -687.564467  
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O -1.266644 -0.765068 1.950270  
O -0.405585 -2.536749 0.234641  
O 2.049560 -1.631850 -0.570617  
O -1.059391 2.517991 -0.560045  
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O 0.864092 0.678109 -1.258779  
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H -2.492994 0.126164 0.766324  
H -1.535825 -1.197809 2.764671  
H -0.919445 -1.492685 1.338832  
H -0.812967 -2.127896 -0.571302  
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H 0.754769 1.033083 0.485324  
H 1.591204 -0.827742 -0.946494  
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H 2.700559 0.916605 -0.307783  
H 2.720032 1.002386 1.185243  
H 2.714600 -1.227023 0.003516

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oh.8h2o, E= -687.563911  
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O 1.829021 0.543007 -1.295502  
O 0.215647 -1.429276 -1.272220  
O 2.223365 1.334577 1.163606  
O 2.958054 -1.530015 0.208785  
O -2.708721 1.411207 -0.300706  
O -2.508787 -0.540730 1.735737  
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  
H 0.821604 -0.620992 -1.434605  
H 0.824449 -2.172770 -1.203882  
H 2.698405 -0.818687 -0.418965  
H 2.214539 -1.552400 0.829292  
H 2.192425 1.140087 0.178246  
H 2.926062 0.755237 1.479426  
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H -2.632839 0.293582 1.238732  
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oh.8h2o, E= -687.563463  
O -0.358277 1.109161 -1.502014  
O 2.014854 0.232885 -1.628373  
O -1.676150 -1.174534 -1.529026  
O -0.667496 -2.177522 0.695982  
O 0.224708 1.851734 1.062014

O -1.640745 0.149585 2.119667  
O 2.113028 -1.761212 0.349183  
O 2.924725 0.887561 0.956833  
O -2.956595 0.953723 -0.229540  
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H -2.684718 0.703318 0.679287  
H -1.093606 -0.368990 -1.677640  
H -2.462545 -0.726513 -1.162706  
H 1.040850 0.609953 -1.609138  
H 2.225694 0.061075 -2.549430  
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H 1.162290 1.601737 1.165194  
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H -0.980869 -3.081798 0.784624  
H -1.034157 -1.841428 -0.179196  
H -0.925472 0.787244 1.879697  
H -1.311174 -0.705162 1.794846  
H -0.506427 1.793094 -2.161487

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oh.8h2o, E= -687.562614  
O -0.226730 1.363777 -1.213241  
O 2.354648 1.755516 -0.207909  
O 2.088538 -0.199943 1.533673  
O -0.383618 -1.132262 1.481917  
O 0.197634 -1.381306 -0.995373  
O -2.569479 -1.714341 -0.319409  
O -3.110144 1.070071 -0.730951  
O -1.423924 1.330907 1.465588  
O 2.939193 -1.102529 -1.096108  
H -0.097630 0.388613 -1.208996  
H 0.659134 1.710055 -0.999654  
H 2.733945 2.546321 0.184422  
H 2.210075 1.108557 0.547981  
H 1.134166 -0.519968 1.615469  
H 2.497695 -0.816635 0.902974  
H -1.963532 -1.531609 0.428210  
H -2.902325 -0.829100 -0.561758  
H -2.799225 1.186643 0.192648  
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H -0.881835 1.559097 0.691273  
H -1.121248 0.402640 1.651869  
H 1.995078 -1.327348 -1.232045  
H 2.960594 -0.136854 -1.148576  
H 0.040927 -1.378085 0.016191  
H -0.643430 -1.742092 -1.315277  
H -0.441112 -1.856233 2.110521

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oh.8h2o, E= -687.562558  
O -0.216161 0.857224 -0.814522  
O 1.210735 -0.533765 1.934462  
O 2.932733 -1.569809 -0.428057  
O 0.071418 -1.700653 -0.394665  
O -3.301198 0.864313 -1.170151  
O -2.698361 -1.651920 0.015296  
O -1.596144 0.514367 1.469105  
O 2.341432 0.880330 -1.589449  
O 1.221010 2.144899 0.885500

H -0.053092 -0.745925 -0.692907  
H 0.973111 -1.947346 -0.663381  
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H 0.584740 1.796062 0.178328  
H 0.663612 2.623660 1.506152  
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H -3.087810 1.264122 -0.318914  
H -3.166542 -0.087932 -0.987701  
H -1.096509 0.654443 0.613771  
H -0.914221 0.175289 2.065894  
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H -2.453530 -1.030031 0.728036  
H 0.734324 -1.010622 1.223886  
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oh.8h2o, E= -687.561377  
O 0.050678 -1.405246 1.980593  
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O 1.169692 2.206295 -0.031307  
O -0.711950 1.420997 -1.851315  
O -0.288864 -1.169925 -1.915108  
O -1.982130 -1.571128 -0.074697  
O -2.661255 0.903257 0.281190  
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H 0.977133 -1.558997 -1.048099  
H -0.369638 -1.642865 -2.746962  
H -0.517356 0.437931 -1.975284  
H -3.612450 0.977673 0.390797  
H -2.460053 -0.084712 0.137171  
H -1.336622 -1.485406 -0.887319  
H -1.392910 -1.759525 0.674043  
H -1.488499 1.426077 -1.270808  
H 0.556947 1.979189 -0.776124  
H -1.268928 1.234046 1.455638  
H 0.228789 1.610437 1.263630  
H 1.946229 1.620265 -0.140217  
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oh.8h2o, E= -687.560990  
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O 2.414349 1.063980 -0.865021  
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O 1.219306 -1.324892 -1.415916  
O 3.192503 -1.172852 0.704181  
O -3.113893 0.457982 -0.343633  
O -2.219281 -1.533470 1.454607  
O -1.620698 -1.799398 -1.334023  
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H -0.568240 2.425000 0.188086  
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H -0.656971 -1.699683 -1.426614  
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oh.8h2o, E= -687.560555  
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O -0.987821 -1.782580 -1.598860  
O 1.467242 -2.193152 -0.560190  
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H 2.471372 -0.704453 -0.568039  
H 1.096492 -0.644648 2.886605  
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H 1.778004 2.784875 -1.453927  
H 1.871057 1.381069 -0.760386  
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H -0.915880 -1.396011 1.443329  
H -1.082767 -0.831806 -1.842479

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oh.9h2o, E= -764.028865  
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O 2.340311 0.447961 1.024526  
O 0.400064 2.229191 1.449052  
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O -1.196257 -1.890062 1.510785  
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O -0.046748 2.332451 -1.431322  
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H 0.005564 -1.890380 -1.634244  
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H 1.621744 -0.247187 -1.755974  
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H -2.030254 -0.626419 -1.173104  
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oh.9h2o, E= -764.027903  
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O 1.958724 -1.618294 -1.170527  
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O -2.398815 0.385077 1.067911  
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H 0.112482 -2.140201 -1.298775  
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H 2.433394 1.373891 2.310516  
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H -1.903706 -0.534453 1.274837  
H -1.541516 -2.427813 1.958008  
H -1.283199 1.777880 1.138486  
H -3.217042 0.390827 1.570382  
H 1.688613 -1.673132 0.730504  
H 0.382670 -1.554267 1.609337

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oh.9h2o, E= -764.027468  
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O 0.357510 -1.960810 -0.990418  
O 1.032029 0.192538 -2.098661  
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H -1.316443 -1.946942 -0.909196

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oh.9h2o, E= -764.026398

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O -2.260376 -1.141669 1.569952  
O 0.448976 -0.259695 1.968081  
O 1.334339 -2.007127 -0.018557  
O 3.124222 -0.171097 -1.275953  
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H -2.295124 2.161555 -0.371659  
H 2.092715 1.715811 0.665650  
H 2.516477 0.746854 1.746679  
H -0.072450 -0.419790 -2.467324

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oh.9h2o, E= -764.025546

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O 0.905593 -2.170958 1.019626  
O 2.378216 -0.071126 1.409141  
O 0.595521 2.353947 -1.305732  
O -2.016563 1.208506 -1.325148  
O -1.797466 -1.359275 -1.302038  
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H -1.783972 -0.398831 1.590847  
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H -0.907669 1.595536 1.562786  
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H 0.906778 -2.669097 -2.089240  
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H 2.512242 0.145547 -0.557996  
H 1.208254 1.597406 -1.486583

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oh.9h2o, E= -764.025304

O -0.137579 0.040712 -1.589312  
O 1.649489 1.536825 -0.400852  
O 3.501087 -0.170165 0.630170  
O -1.517029 1.200848 0.288642  
O -3.784027 -0.280835 0.515638  
O 1.860647 -1.820223 -1.124916  
O -1.854506 -1.979168 -0.869460  
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  
H -0.655728 -2.411113 0.451606  
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  
H -0.551784 3.805136 -1.054590  
H -0.285358 0.235551 -2.518797

29

oh.9h2o, E= -764.024443

O -0.455856 -2.660241 0.591589  
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  
H -0.084709 -2.158735 -0.182520  
H 0.317731 -2.739084 1.165447  
H 0.775944 0.336410 -1.314341  
O 0.940198 1.372722 -1.183081  
H 1.164435 1.743718 -2.041185  
O 2.213953 -1.248773 0.942979  
H 1.851508 -0.506893 1.463727  
H 1.699139 -1.205834 0.105775  
O 3.768059 0.655545 -0.588488  
H 2.896567 1.051293 -0.743698  
H 3.550040 -0.085281 0.002888  
O 0.787003 1.108138 1.742653  
H 0.955420 1.317046 0.812555  
H -0.066976 0.604862 1.766178  
O -1.145294 2.773351 -0.008936  
H -0.843630 2.665587 0.902763  
H -0.446652 2.314156 -0.523493

29

oh.9h2o, E= -764.024150

O -2.785211 -0.609105 -1.282161  
O -3.254865 1.760546 0.307783  
O -0.964204 0.583905 1.086360  
O -0.027280 0.235715 -1.413275  
O 2.796936 0.007131 -1.619012  
O 2.499528 -1.279571 0.949437  
O 0.463951 -2.195860 -0.408147  
O -1.946847 -2.042580 0.994352  
O 1.551133 1.176986 2.013791  
O 1.578951 2.322386 -0.523307  
H -1.833221 -0.396711 -1.384590  
H -3.142754 0.172310 -0.822183  
H -2.921150 2.495234 -0.216819  
H -2.452711 1.422735 0.776543  
H -0.642585 0.497819 0.149764  
H -0.161782 0.832122 1.600371  
H 1.815808 -0.024354 -1.679122  
H 2.973729 -0.465905 -0.789574  
H 1.698253 -1.692773 0.493601  
H 2.967765 -2.000200 1.379036  
H -0.353019 -2.338100 0.116399  
H 0.262293 -1.379712 -0.940022  
H 1.668033 1.723723 1.205296  
H 1.950799 0.318757 1.776002  
H -1.625503 -1.175086 1.311381  
H -2.448005 -1.774487 0.198190  
H 0.863027 1.709527 -0.821154  
H 2.350325 1.867501 -0.902885  
H -0.266040 0.531168 -2.296800

29

oh.9h2o, E= -764.023469

O -0.301493 -1.459751 -1.123917  
O -2.813474 -1.402823 -0.697077  
O -2.654765 -0.470279 1.740536  
O 0.156308 -0.641950 1.286348  
O -2.355100 1.986397 0.351325  
O 0.519966 1.869700 0.216914  
O -0.975972 1.006168 -2.026146  
O 3.303294 1.393771 0.070168  
O 2.507697 -0.989425 -1.336472

O 2.925003 -1.106035 1.468945  
H -0.705281 0.071109 -1.852723  
H -1.654014 1.219699 -1.361801  
H -1.802064 -1.501718 -0.901366  
H -3.106119 -0.703881 -1.291944  
H 0.023652 -1.086224 0.384845  
H -0.719226 -0.656502 1.706450  
H 1.528445 -0.989494 -1.318637  
H 2.782950 -0.073345 -1.145974  
H 3.327112 0.694723 0.750437  
H 2.402966 1.764796 0.146768  
H 0.236491 1.685176 -0.702344  
H 0.424219 0.997380 0.668942  
H -1.419816 2.212442 0.504535  
H -2.536453 1.261098 0.974215  
H -2.795223 -0.877988 0.830610  
H -3.306736 -0.860036 2.328545  
H 2.900763 -1.349452 0.522521  
H 1.978320 -0.995542 1.674124  
H -0.051706 -2.298420 -1.522198

29

oh.9h2o, E= -764.023179

O -0.269874 2.146877 1.313134  
O -2.456970 0.663448 1.162837  
O -1.444296 -2.043129 1.259996  
O 1.319399 -1.627168 1.614124  
O 1.865214 0.854575 1.511624  
O 2.414548 0.699771 -1.335813  
O 1.558903 -1.816949 -1.129512  
O -1.153065 -1.779316 -1.578499  
O -2.069316 0.610155 -1.514443  
O 0.011363 2.347791 -1.289603  
H -1.648765 1.242155 1.315740  
H -0.331616 2.952753 1.832495  
H -2.170526 -0.245408 1.369195  
H -0.506770 -1.914476 1.500905  
H -1.431261 -2.080522 0.286905  
H 1.828661 -2.021997 2.326350  
H 1.525997 -0.613399 1.623338  
H 2.249035 0.981799 0.629503  
H 0.973757 1.425203 1.499195  
H -0.102174 2.382161 -0.285403  
H 0.843880 1.865532 -1.416705  
H -2.358140 0.673929 -0.563552  
H -1.329576 1.269174 -1.569713  
H -1.505630 -0.814283 -1.601694  
H -1.646404 -2.269612 -2.240983  
H 1.548815 -1.912670 -0.153201  
H 0.611848 -1.848978 -1.388028  
H 2.095124 -0.246017 -1.317884  
H 3.146498 0.726206 -1.957222

29

oh.9h2o, E= -764.022728

O -2.528415 -0.628149 -1.270289  
O -3.219041 1.958161 -0.141894  
O -0.667037 1.531306 0.563750  
O 0.120709 0.077107 -1.445659  
O 2.562929 1.010324 -0.751144  
O 3.548953 -1.576839 -0.108195  
O 0.899272 -1.968756 0.034866

O -1.982036 -2.684298 0.477310  
O -0.568899 -0.844676 2.122160  
O 1.734209 2.945916 0.875076  
H -1.571416 -0.386295 -1.363107  
H -2.936382 0.144997 -0.842487  
H -3.106489 2.442404 -0.965690  
H -2.304361 1.912755 0.236351  
H -0.359877 1.058300 -0.271754  
H 0.070666 2.123184 0.814439  
H 1.677667 0.653506 -1.040648  
H 3.056051 0.224464 -0.447671  
H 2.588960 -1.813360 0.018819  
H 3.776920 -1.961778 -0.959816  
H 0.572885 -1.598143 0.885129  
H 0.606905 -1.286379 -0.637218  
H 1.776240 3.703538 0.284118  
H 2.152364 2.205516 0.351999  
H -0.675601 0.028820 1.694734  
H -1.281833 -1.405150 1.759167  
H -1.065811 -2.824977 0.191375  
H -2.318393 -2.014716 -0.161958  
H 0.136350 0.232553 -2.393627

29

oh.9h2o, E= -764.022492

O 2.476621 0.289707 -1.616522  
O 3.532884 -0.858578 0.733098  
O 1.050517 -1.953083 0.617768  
O -0.109840 -0.571237 -1.436926  
O -2.919362 0.508709 -1.585793  
O -2.859648 1.707470 1.008739  
O -0.236522 1.352072 0.365846  
O -1.271752 -0.728926 1.997350  
O 2.480002 2.054739 0.348732  
O -2.223599 -1.941561 -0.311377  
H 1.537641 -0.042971 -1.586079  
H 2.983375 -0.329721 -1.056420  
H 3.371694 0.039979 1.049470  
H 2.658551 -1.312724 0.816987  
H 0.667116 -1.568086 -0.207706  
H 0.393532 -1.746302 1.302381  
H -1.959636 0.343462 -1.623186  
H -3.044527 1.001464 -0.751903  
H -1.910065 1.847948 0.809865  
H -2.826472 0.936313 1.592881  
H 0.659309 1.715614 0.492494  
H -0.186546 0.744020 -0.422096  
H -1.396378 -1.631028 -0.754537  
H -2.870588 -1.324524 -0.692130  
H 2.521071 1.500336 -0.484509  
H 2.780423 2.934706 0.105488  
H -0.820369 0.009612 1.544198  
H -1.715483 -1.222770 1.271347  
H -0.197052 -0.769832 -2.373873

29

oh.9h2o, E= -764.022314

O -2.135551 -1.538671 -0.972773  
O 0.288868 -1.994229 -0.851392  
O 1.179022 -0.929444 1.937814  
O 2.862458 -1.189101 -0.118848  
O 0.388616 0.731898 -1.475137

O 2.949874 1.488727 -0.875077  
O 0.747943 1.758807 1.056108  
O -2.189794 1.798366 1.189460  
O -1.856605 -0.927023 1.575867  
O -2.263117 1.037111 -1.578714  
H -0.766032 -1.898258 -1.019979  
H 0.324928 -2.114893 0.104910  
H -0.567533 0.949338 -1.663004  
H 0.389417 -0.236045 -1.302480  
H -2.358329 0.051437 -1.428647  
H -2.387685 1.424450 -0.689713  
H -2.044577 -1.220629 0.629895  
H -0.897304 -0.988275 1.681771  
H -2.176668 0.841445 1.423650  
H -1.253360 2.048875 1.251203  
H 0.851624 0.945598 1.579256  
H 0.526304 1.419250 0.156660  
H 1.535515 -1.286293 2.755962  
H 1.888253 -1.033937 1.242174  
H 3.043290 -0.272784 -0.428362  
H 2.162295 -1.530376 -0.708321  
H 2.122930 1.360477 -1.385191  
H 2.599653 1.855610 -0.047278  
H -2.766430 -2.206509 -1.250980

29

oh.9h2o, E= -764.021692

O -0.186752 0.175018 -1.291555  
O 0.821022 -2.306503 -0.732019  
O 2.199976 -1.283369 1.608585  
O 3.130200 -0.009187 -0.445398  
O 1.607375 1.932756 -0.941881  
O -0.226620 0.052195 1.541766  
O -0.305006 2.819034 0.747892  
O -2.446568 1.579595 -0.588612  
O -2.000002 -2.307709 -1.017072  
O -2.898134 -0.645694 1.140281  
H 0.528964 -1.399534 -0.975930  
H 1.229089 -2.209631 0.143211  
H 0.525354 0.919311 -1.289595  
H 1.884072 2.517497 -1.652084  
H -2.768954 0.924809 0.063242  
H -1.824481 2.162538 -0.097562  
H -1.814007 -1.527355 -1.555810  
H -1.099058 -2.606344 -0.785623  
H -2.725506 -1.329262 0.464774  
H -2.016595 -0.492807 1.531134  
O 0.590266 -0.405018 1.815280  
H -0.173829 0.067273 0.561033  
H 2.883029 -1.513250 2.243024  
H 2.637901 -0.730447 0.879833  
H 2.569179 0.858533 -0.640669  
H 2.860317 -0.630118 -1.132780  
H -0.241267 2.074461 1.366869  
H 0.443422 2.629983 0.117044  
H -1.051829 0.640278 -1.231284

29

oh.9h2o, E= -764.021605

O -1.144918 -1.547646 -0.398315  
O -2.272671 -0.137991 1.417827  
O 1.230977 -2.362312 -1.405623

O 1.885547 0.287436 -1.528582  
O -0.225079 1.677465 1.244748  
O 2.345158 2.732433 0.097366  
O 2.076807 0.050830 1.207014  
O -0.804230 0.870414 -1.433696  
O 0.658858 -2.478869 1.503023  
O -3.698657 1.068926 -0.813581  
H -0.074392 -2.212131 0.903469  
H 1.170018 -1.666479 1.635772  
H 0.303164 -2.084229 -1.173737  
H 1.529730 -2.705677 -0.550422  
H -0.983116 -0.071582 -1.135329  
H -0.667881 1.346345 -0.592417  
H -1.834530 -0.757011 0.718337  
H -2.374305 -0.665264 2.215046  
H 2.367658 2.078146 -0.618347  
H 1.418521 2.743214 0.379332  
H 0.481804 1.015699 1.372733  
H -1.047237 1.184271 1.458706  
H 2.601541 0.838900 1.402184  
H 2.030670 0.062046 0.220022  
H 1.846520 -0.690423 -1.653149  
H 0.951230 0.565977 -1.675237  
H -2.844331 1.128449 -1.270556  
H -3.455535 0.688065 0.044947  
H -1.833866 -2.083794 -0.802811

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oh.10h2o, E= -840.490439  
O -2.757824 1.409235 -0.633138  
O -2.840321 0.165862 1.668534  
O -1.991064 -0.820202 -1.942942  
O -2.104334 -2.341962 0.447887  
O 0.609024 -1.634543 0.446803  
O 3.245778 -2.170127 0.674655  
O 0.691991 -0.242394 -1.753561  
O -0.062388 2.041189 -0.753476  
O 3.104652 0.396895 -0.632359  
O 2.229418 2.531937 0.810507  
O -0.097787 0.737431 1.701924  
H -2.597475 0.626577 -1.225724  
H -2.125554 -1.479266 -1.232442  
H -2.438737 -1.595975 0.975551  
H -2.878120 0.684737 0.802682  
H 0.254604 1.232944 -1.267971  
H 0.648305 -1.226343 -0.475549  
H 0.448026 -0.851834 1.020418  
H -0.183414 1.210234 0.842257  
H 2.668886 1.781945 0.337163  
H 3.330086 -0.401077 -0.121759  
H 1.728030 2.100657 1.515247  
H -1.901470 1.881042 -0.666792  
H -1.128827 -2.265306 0.511618  
H 0.955199 -0.448079 -2.654347  
H -1.018766 0.568273 1.970852  
H 0.737736 2.487408 -0.415451  
H 2.258794 -2.065389 0.690713  
H 3.408941 -2.776075 -0.054588  
H 2.250900 0.167612 -1.084790  
H -1.017142 -0.633254 -1.921922  
H -3.617160 0.414595 2.176161

32

oh.10h2o, E= -840.490063  
O 3.019833 0.657174 -0.014806  
O 1.890458 -0.803910 2.076836  
O 1.492357 -2.515661 -0.108883  
O 1.137939 -0.511670 -1.635411  
O -2.804481 1.152095 -1.216044  
O -3.308016 1.134737 1.621115  
O -0.151997 1.505882 -0.579987  
O -0.832707 -0.024203 1.624749  
O -1.226604 -2.477748 0.506408  
O 2.080437 3.142522 -0.102792  
O -1.551663 -1.292675 -1.939434  
H 2.417950 0.219870 -0.669537  
H 2.757162 0.240826 0.835132  
H 0.978367 -0.460694 2.143018  
H 1.809531 -1.540064 1.438477  
H 1.385594 -1.753291 -0.798512  
H 2.140321 -3.130787 -0.460621  
H -1.895316 1.480983 -1.061384  
H -3.169441 1.070688 -0.315606  
H -3.094621 2.051950 1.819312  
H -2.453583 0.654912 1.756529  
H 0.494176 2.214635 -0.392543  
H 0.355442 0.794746 -1.077540  
H -0.615240 -0.992014 -1.904057  
H -2.090747 -0.491040 -1.779093  
H 2.527560 2.252972 -0.004506  
H 2.424918 3.500893 -0.926112  
H -0.550220 0.517703 0.851472  
H -1.016856 -0.931583 1.266585  
H -0.297871 -2.737909 0.360470  
H -1.508451 -2.167933 -0.387032  
H 1.436875 -0.527210 -2.548468

32

oh.10h2o, E= -840.488586  
O -0.106148 0.060477 -1.245077  
O 3.338226 0.072945 0.143958  
O -1.736449 1.819042 0.091954  
O 0.675059 2.749624 1.210164  
O 1.687817 1.864437 -1.234652  
O 1.852198 -1.897411 -1.292976  
O 0.744350 -0.213541 1.413193  
O -3.167311 0.107534 -1.929866  
O 0.595138 -2.899517 0.950607  
O -1.859172 -1.779305 -0.076955  
O -2.075874 -0.045846 2.114607  
H 2.635783 -0.010319 0.812420  
H 2.998001 0.788955 -0.424824  
H 1.131083 -1.238531 -1.427477  
H 2.562967 -1.361724 -0.892143  
H -3.039870 0.868336 -1.346515  
H -2.973238 -0.658743 -1.362969  
H 0.388066 -0.076238 0.512063  
H 0.774747 -1.200857 1.472465  
H -1.141753 1.207408 -0.411645  
H -1.097351 2.414958 0.528046  
H 0.952027 1.147573 -1.348470  
H 1.754764 2.341728 -2.065506  
H 0.804727 1.906896 1.669101  
H 1.122059 2.610088 0.350261

H -1.169816 -1.203812 -0.479788  
H -2.092048 -1.308898 0.751626  
H -1.113857 -0.101910 2.241006  
H -2.152133 0.703715 1.484920  
H 1.111233 -2.748297 0.124207  
H -0.331828 -2.840331 0.655288  
H -0.706232 0.052473 -2.001717

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oh.10h2o, E= -840.486404  
O -2.646397 0.051843 1.853407  
O 0.064295 0.032673 1.646093  
O 0.233646 2.472258 0.550725  
O -2.472418 1.745234 -0.329558  
O -1.537204 -0.390799 -1.709362  
O 0.077987 -1.878279 -0.349863  
O -2.885482 -1.945940 -0.111374  
O 0.601770 1.340348 -2.006478  
O 3.085941 0.548045 -1.061795  
O 2.876778 -2.118672 -0.043001  
O 2.899165 0.229705 1.716790  
H -2.707126 0.762912 1.174143  
H -2.819463 -0.752517 1.325074  
H 2.978032 -1.560174 0.748405  
H 3.125282 -0.424828 -1.027214  
H 2.233089 0.763215 -1.500778  
H 1.913378 -2.151436 -0.192645  
H -0.437185 -1.313438 -1.017220  
H 1.949746 0.202937 1.920183  
H 2.957212 0.552284 0.791963  
H 0.465112 1.894380 -1.216615  
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H -2.455913 -1.326534 -0.793601  
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H -0.582784 -2.512520 -0.045534

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O 1.144503 2.465865 -0.635799  
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O 2.602969 -0.944085 -1.390584  
O 1.527111 -2.983787 0.330791  
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H -3.675371 -0.645652 -1.910246  
H -3.268462 -0.120292 -0.525864  
H -1.282895 0.706632 -0.424154  
H -1.913148 1.965646 0.283893

H 1.693597 -0.571121 -1.422925  
H 2.459938 -1.788878 -0.924939  
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H 0.820505 -0.166381 0.512140  
H -0.136698 3.211453 0.164453  
H -1.233472 4.226014 -0.228917  
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  
H 2.748974 0.671026 1.145167  
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oh.10h2o, E= -840.486191  
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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  
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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 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  
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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  
H -2.580863 0.243680 1.277448  
H -1.211647 0.949213 1.696889

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oh.10h2o, E= -840.485318  
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O -2.027992 1.796037 1.500870  
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O -0.091513 -2.600410 1.456382  
O 1.692994 -0.725862 1.533680  
O 0.205203 -2.550195 -1.264761  
O 0.335225 1.021167 -1.778864



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H 0.397637 1.350950 -0.858375  
H -2.332723 0.793492 -1.251230  
H -1.735976 2.189034 -1.520158  
H -2.215426 -1.005900 0.130475  
H -2.274618 -0.191446 1.451510  
H -0.501764 -1.860334 -1.371616  
H 1.043143 -2.081062 -1.413025  
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H 2.644951 2.091822 0.441504  
H 3.426014 1.083725 -0.394222  
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H 2.381649 -0.848461 2.191851  
H -0.951585 -2.111505 1.479759  
H 0.027924 -2.784013 0.492694  
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oh.10h2o, E= -840.483002  
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O 1.925012 -1.929926 -1.242433  
O -3.502005 -0.113792 0.115383  
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H 3.060948 0.994817 -1.845314  
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H -1.263781 -0.749686 1.817824  
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oh.10h2o, E= -840.480735  
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O 1.408250 -1.851240 1.708854  
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H 1.282802 2.739127 -0.066723  
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oh.10h2o, E= -840.480518  
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O -3.088048 1.749039 -0.422515  
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O 0.659827 -1.235391 -0.887062  
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oh.10h2o, E= -840.479831  
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oh.11h2o, E= -916.947309  
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H -2.845511 1.278801 0.681350  
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H -3.854917 -2.412310 -0.241719  
H 1.750180 -2.095011 0.209910  
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H 0.951726 -0.221478 -2.2114093  
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oh.11h2o, E= -916.947134  
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O 1.836854 1.845709 -1.350506  
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O 0.949409 -0.065671 1.342691  
O -1.631904 -0.559387 2.043001  
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H -3.360761 -0.310838 -0.719551  
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H 1.435162 -1.354451 -1.336273  
H 1.990044 -2.516935 -0.507606  
H 1.171054 -2.076080 1.414805  
H 0.183603 -3.041138 0.759240  
H 0.069569 -0.190275 1.775714  
H 0.736769 -0.085065 0.388764  
H -0.639570 3.312569 0.538214  
H -1.233766 3.938410 -0.741803  
H -1.983828 0.094736 1.404077  
H -1.612534 -1.367006 1.492764

H 1.149072 1.141622 -1.400015  
H 2.622774 1.362319 -1.019185  
H 3.276454 -0.673826 -0.481841  
H 3.067864 0.161450 0.781545  
H 1.329230 2.623811 0.137134  
H 0.920469 1.933478 1.426154  
H -0.141600 -0.296769 -2.242972

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oh.11h2o, E= -916.946506  
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O -1.543284 1.830355 -0.187629  
O -0.246731 -0.197450 -1.276443  
O 2.005211 1.316184 -1.315702  
O 3.593946 -0.838013 -0.522574  
O 2.425014 1.297037 1.557465  
O 1.430654 -2.398501 -1.170401  
O -0.394293 -3.315737 0.831462  
O 0.467197 -0.681727 1.447171  
O -2.044813 0.206031 2.027511  
O 0.757445 3.374191 0.173548  
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H -3.133027 -0.921752 -0.568364  
H -3.880306 0.988471 -2.049927  
H -3.156861 1.355066 -0.743142  
H -1.023492 1.096180 -0.634109  
H -0.890986 2.547142 -0.043784  
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H 0.937780 -2.960915 -0.544301  
H -0.048118 -2.527297 1.290825  
H -1.242444 -3.007387 0.474587  
H -0.371416 -0.332111 1.833919  
H 0.346912 -0.559142 0.487842  
H 1.265790 2.884087 -0.500562  
H 1.127747 3.020323 0.997138  
H -1.958399 0.958999 1.407023  
H -2.364909 -0.503458 1.436152  
H 1.177272 0.767177 -1.333497  
H 2.725089 0.652564 -1.292169  
H 2.895303 -1.515456 -0.687687  
H 3.474478 -0.561819 0.395493  
H 2.406033 1.375041 0.587609  
H 1.764297 0.594266 1.724390  
H -0.442692 -0.235759 -2.218033

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oh.11h2o, E= -916.944841  
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O -2.239828 2.572862 -0.374438  
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O 3.038350 1.831124 -0.049192  
O 3.365918 -0.142847 1.702198  
O -2.495153 -1.067866 -1.410618  
O -0.390019 0.729131 -2.150335  
O 3.346062 -0.698373 -1.214094  
O 0.854616 -1.730499 -1.750560  
O -0.608590 -2.155188 0.266510  
O -2.201059 -1.039117 2.253381  
O 0.552359 -0.354040 1.837378  
H -3.480005 -0.102731 -0.241415  
H -3.310304 0.062281 1.265178

H 3.958560 0.045578 2.434721  
H 3.293210 0.698049 1.167184  
H 3.493580 -0.929845 -0.286373  
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H 1.520423 -0.418423 1.919696  
H 0.240737 -1.100277 1.248837  
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H 0.263222 -1.946593 -0.913694  
H -0.052515 1.147284 -1.332138  
H 0.120617 -0.104180 -2.198232  
H -2.052094 2.229357 -1.257452  
H -2.843233 1.890143 0.020393  
H -1.436882 -0.573268 2.620760  
H -1.782162 -1.523476 1.503032  
H -1.909362 -1.581207 -0.804936  
H -1.896056 -0.379247 -1.756913  
H -0.579513 2.275910 0.284134  
H 0.296938 1.106026 0.926632  
H -0.561846 -3.075302 0.542669  
H 0.643152 -2.391287 -2.415507

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oh.11h2o, E= -916.944432  
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O -2.045777 1.860910 -1.286521  
O -0.354031 1.568706 0.838908  
O -1.534520 -1.700865 -0.992777  
O 0.355085 0.296396 -1.803837  
O -2.939167 0.177196 1.883354  
O -0.482136 -1.092884 1.454553  
O 1.834706 0.076782 2.372851  
O 1.004890 -2.901781 -0.043633  
O 2.557561 -1.199209 -1.611155  
O 3.650104 0.497621 0.273696  
O 1.897932 2.599571 -0.476253  
H -3.163626 -0.844112 -0.963222  
H -3.751336 -0.047252 0.200839  
H 3.207649 1.324447 -0.000336  
H 3.082471 -0.655288 -0.979062  
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H 3.145076 0.234903 1.070455  
H 1.057301 -0.436448 2.036355  
H 1.147702 2.345114 0.100443  
H 1.620117 2.282452 -1.345294  
H 0.266253 -3.067136 -0.645403  
H 0.603655 -2.253598 0.583500  
H 0.341342 0.558576 -0.871288  
H 1.188509 -0.248879 -1.882486  
H -1.421776 1.450384 -1.902507  
H -2.784150 1.210426 -1.194861  
H -2.612545 1.082125 1.948150  
H -2.114006 -0.345388 1.739307  
H -1.258855 -1.553620 -0.053086  
H -0.948313 -1.093647 -1.483208  
H -1.067401 1.741061 0.177713  
H -0.437758 0.628145 1.124060  
H -0.644975 -1.626637 2.239659  
H 1.492601 0.976067 2.432541

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oh.11h2o, E= -916.944120

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O -1.425713 -0.634516 2.086225  
O 1.416439 -1.991024 -0.118056  
O -0.994399 -3.062376 0.736565  
O -1.873355 -1.515505 -1.445989  
O -3.402903 -0.034828 0.085541  
O -1.918032 2.071514 -1.134465  
O 0.594475 1.151344 1.111209  
O 2.613828 -0.367111 -2.337878  
O -0.704467 3.607316 0.691904  
O 3.270132 1.247377 -0.132527  
O 2.782676 -0.631397 1.863436  
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H -2.146349 -0.313951 1.515764  
H -1.199887 1.395475 -1.281843  
H -2.631765 1.555861 -0.724024  
H 2.460763 -1.193271 -1.857733  
H 2.937350 0.244688 -1.641923  
H 0.348865 0.778849 0.208859  
H 0.180864 2.037179 1.150087  
H 0.878327 -1.230928 -0.434507  
H 0.730094 -2.602069 0.225531  
H -1.029446 -0.814813 -1.424174  
H -2.064064 -1.711913 -2.366816  
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H -1.237105 3.118789 0.006549  
H -0.102463 4.163013 0.187592  
H -4.275496 -0.401294 0.251399  
H -2.938167 -0.657966 -0.546483  
H 0.641770 0.163745 -1.878011

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oh.11h2o, E= -916.943411  
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H 0.457667 2.977645 -0.181741  
O 1.940994 -0.529555 2.089201  
H 1.046384 -0.173883 1.913042  
H 2.532109 0.103732 1.608071  
O 1.740236 -2.632090 0.495560  
O 3.322038 1.142876 0.432491  
O -1.341671 2.858095 0.829156  
O -2.468101 1.163503 -1.340842  
O -0.495829 0.344563 1.091824  
O 0.116710 0.330989 -1.657824  
O 2.651084 -0.759880 -1.475156  
O -0.594494 -2.233965 -1.149134  
O -3.172479 -1.453953 -0.628403  
O -2.790595 -0.907150 1.926573  
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H -3.407082 -0.193730 2.118491  
H -3.066416 -0.532973 -0.951444  
H -2.305671 -1.878890 -0.831494  
H -1.519319 0.912729 -1.495428  
H -2.418388 1.872381 -0.684454  
H -0.336835 0.165157 0.143007  
H -1.271531 -0.193461 1.378749

H 0.097862 0.411320 -2.617026  
H -0.294230 -1.330491 -1.428477  
H 0.087041 -2.529919 -0.522007  
H 1.751776 -0.362110 -1.578200  
H 2.489411 -1.558426 -0.946417  
H 2.089996 -3.422647 0.914411  
H 1.845609 -1.884479 1.157383  
H 2.648350 1.802662 0.161952  
H 3.283575 0.487451 -0.299129  
H -1.411173 3.321668 1.668262  
H -1.009543 1.945845 1.041981

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oh.11h2o, E= -916.942841  
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O -1.426773 -1.583405 -0.313134  
O 0.253118 -3.699217 -0.498636  
O 2.018815 -2.157943 0.561875  
O 2.927554 1.457941 0.696968  
O -0.388366 1.871586 -0.547479  
O -1.649933 0.312294 -2.505541  
O -1.648895 -0.386268 2.580106  
O 1.835984 3.531447 -0.574485  
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H 3.275904 -0.602407 -1.676431  
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H -0.741909 -0.998091 0.065185  
H -0.957791 -2.448789 -0.416049  
H 1.212415 -0.985014 0.924798  
H 2.462730 -2.548275 1.320715  
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H 1.002104 -3.152038 -0.062743  
H -1.896101 1.962428 0.565010  
H -3.222814 1.183237 0.501991  
H -3.343941 0.255555 -1.516624  
H -3.204771 -0.788455 -0.448580  
H 2.347123 2.790090 -0.145219  
H 1.790684 4.220017 0.095570  
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H 0.038788 -0.195625 1.804764

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oh.11h2o, E= -916.942217  
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O 1.385374 3.283601 -0.289675  
O 2.864611 -0.617883 -1.244941  
O 3.386645 1.607268 0.279136  
O 1.612190 0.299592 1.981868  
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O -2.538364 -0.865416 -1.604455  
O -2.949103 1.753893 -0.635402

O -4.238856 0.333824 1.552254  
O -1.904778 -1.027577 1.004625  
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H 2.705288 -3.031381 1.495508  
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H -3.441012 1.476785 0.157420  
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H -2.800200 0.073932 -1.530905  
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H -4.845366 -0.178821 1.007707  
H -3.414263 -0.204709 1.556939  
H -2.220401 -1.076461 0.061153  
H -1.273621 -0.286980 0.971690  
H 2.923368 1.206753 1.045980  
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oh.11h2o, E= -916.942106  
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O 0.935435 0.090937 2.424850  
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O 4.237011 -0.083077 -0.677184  
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O 0.862414 2.363581 1.128030  
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H -3.510577 -0.032935 0.388864  
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H -0.109853 -1.886985 0.202286  
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H -0.832740 1.415543 -1.376135  
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H -3.068927 1.892030 1.435869

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oh.11h2o, E= -916.939750  
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O 1.262320 -1.032695 2.256501  
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H -2.176278 0.690054 -1.565184  
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H 1.206610 1.660230 -1.564691

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H 1.382706 2.825645 0.495251  
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H 0.457893 2.188265 -1.428182  
H -2.365623 -0.300240 -2.511379

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oh.11h2o, E= -916.938955  
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O 2.676966 -1.807382 -0.445310  
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O -2.102841 1.499810 -1.864831  
O -1.620762 -1.313223 -1.370558  
O 1.038300 -0.839055 -2.484613  
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O 4.202723 0.336861 0.871902  
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H 0.056599 1.257042 0.531512  
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H -1.136978 -1.271435 3.274506  
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H 0.855100 0.752442 -1.713602  
H -0.302503 1.768036 -1.571026  
H -2.198343 -1.321654 -0.543314  
H -1.747545 -0.410938 -1.712425  
H 3.652437 -0.335640 0.441237  
H 1.673805 2.299860 1.404480  
H 3.657196 1.144614 0.860987  
H 1.910023 2.399558 -0.079731  
H 1.729157 -1.230415 -1.914526

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oh.11h2o, E= -916.937089  
O 0.115144 -2.745635 -0.972573  
O 2.600208 -1.735760 -0.797922  
O -1.749139 -2.438576 1.077578  
O -3.199239 -0.876097 -0.265936  
O -2.972653 1.299300 0.996685  
O -1.459007 2.644480 -0.998398

O -0.904204 -0.158790 -1.298541  
O 1.690295 0.542932 -2.237565  
O 1.381831 2.792477 -0.529301  
O 1.874892 1.520490 1.918254  
O 3.763646 -0.577177 1.656757  
O -0.537460 0.053971 1.462554  
H 1.725153 -2.201907 -0.763871  
H -0.251924 -1.910850 -1.329641  
H -0.835065 -0.871199 1.560635  
H -1.352823 0.592314 1.517404  
H -2.030933 2.422176 -0.241852  
H -1.301082 1.772168 -1.398916  
H -0.432656 -2.881530 -0.174861  
H -2.227526 -2.972043 1.716640  
H -3.687212 1.484064 1.610677  
H -3.212233 0.439669 0.475116  
H 3.202175 -2.328582 -1.256561  
H -3.942237 -1.136226 -0.814326  
H -2.443924 -1.896456 0.527589  
H 0.751945 0.296641 -2.203716  
H 1.602588 2.082288 -1.164471  
H 0.416071 2.901763 -0.612179  
H -1.849322 -0.439247 -1.088687  
H -0.547333 0.009434 -0.398864  
H 3.367554 -0.988136 0.874482  
H 1.083036 0.957314 1.909536  
H 3.209352 0.215401 1.805202  
H 1.786544 2.047853 1.095478  
H 2.135344 -0.167830 -1.737541

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oh.11h2o, E= -916.937069  
O 1.837219 1.710809 -0.657092  
O 3.684380 0.074284 -1.222903  
O -0.412350 0.584606 -1.237086  
O -3.350808 -2.120178 -0.293822  
O -1.070795 -2.049370 -1.716063  
O -0.483623 -0.321973 1.357455  
O 0.397512 -2.819016 0.516229  
O 3.040694 -1.793217 0.514908  
O 2.046485 0.642516 1.817337  
O -0.190356 3.642536 0.291683  
O -3.178864 0.220999 1.180741  
O -2.589265 2.194343 -0.492310  
H 0.472451 1.074844 -1.130068  
H -1.131585 1.239612 -1.207678  
H 0.336881 0.076071 1.732625  
H -0.470288 -0.018890 0.416795  
H 2.032741 1.178806 0.982374  
H 2.479474 -0.188014 1.563117  
H 0.443751 2.912162 0.197384  
H -1.052745 3.246171 0.092021  
H -3.364530 2.497718 -0.971104  
H -2.897097 1.489262 0.148474  
H -3.343226 -0.590263 0.648510  
H -2.272094 0.080578 1.525923  
H -3.124507 -2.810813 0.337582  
H -2.557454 -2.081578 -0.898092  
H -0.471629 -2.450326 -1.048584  
H -0.802667 -1.105638 -1.724749  
H 0.025427 -2.033164 0.971995  
H 1.343704 -2.596203 0.440415

H 3.804144 -2.352468 0.681161  
H 3.304665 -1.156415 -0.215916  
H 2.907592 0.756956 -1.059550  
H 4.467293 0.533692 -0.903701

H 2.027873 2.567186 -1.051549