

The Many-Body Expansion Combined with Neural Networks

Supplementary Material

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Neural networks

Neural networks (NNs) consists of three types of layers: an input layer, hidden layers and an output layer. Each layer contains a certain number of neurons. The value of the neurons in the input layer is simply the input for the NN and the value of a neuron in the hidden layers and output layer is determined by the value of the neurons in the previous layer via the function:

$$y_{i,m} = f(b_m^i + \sum_n w_{i-1,n}^{i,m} y_n^{i-1}) \quad (1)$$

where $y_{i,m}$ is the value of the m^{th} neuron in the i^{th} layer, f is the activation function, usually $f(x) = \max(0, x)$ or $\tanh(x)$, b_m^i is the learned bias for the neuron, y_n^{i-1} is the value of the n^{th} neuron in the $i - 1^{th}$ layer and $w_{i-1,n}^{i,m}$ is the learned weight that connects these two neurons. With the function above, the input values are non-linearly transformed in the

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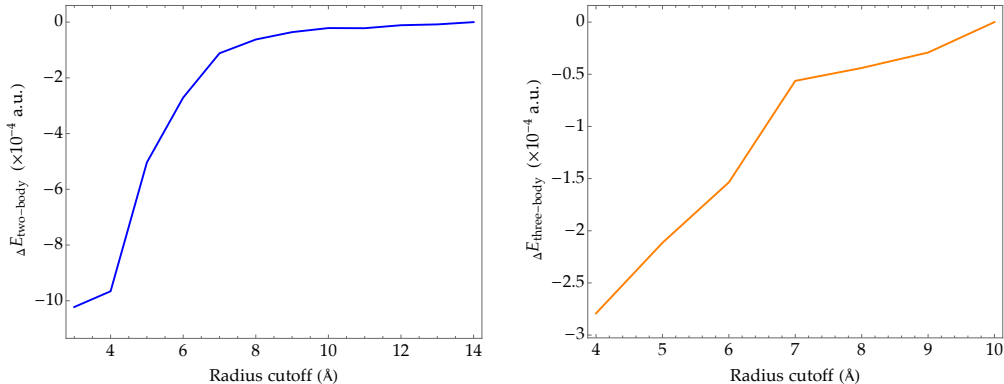


Figure 1: Change in energy per molecule of the two-body (left panel) and three-body (right panel) contributions to the total energy as the cutoff distance is increased in a random cluster of 108 methanol molecules.

hidden layers to approximate the target value. The performance of a NN largely depends on both the size of the training data and the layer structure of the NN. The optimal layer structure is mostly found by trial and error.¹ Small networks may not have enough complexity to model the training data, while large network may suffer from overfitting the training data, which can be prevented by applying regularization.²

Radius cutoff of two-body energy and three-body energy

In order to choose to reasonable radius cutoff, the convergence of two-body energy and three-body energy with respect to the radius cutoff is studied. Figure 1 shows the two-body energy and three-body energy with respect to the radius cutoff of a cluster of 108 methanol molecules which is randomly sampled from an MD trajectory at 330 K. As it is shown in the Figure 1, the convergence of the two-body energy is not achieved until the cutoff reaches 8 Å. The three-body energy requires a larger cutoff to converge than the two-body energy and a cutoff of at least 10 Å is required.

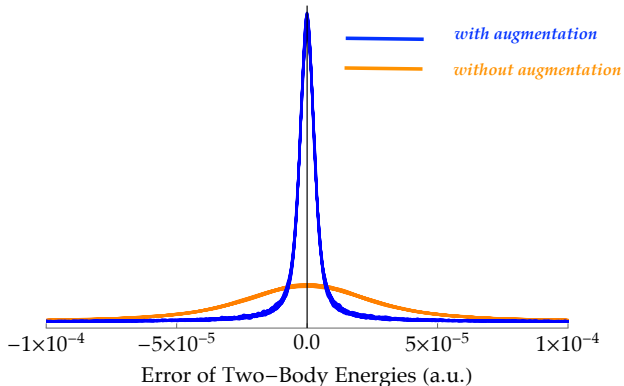


Figure 2: Histogram of the two-body energy error of the neural network trained with data augmentation (blue) and the neural network trained without data augmentation (orange). The errors of the neural network trained without augmentation is much more spread over the axis, while the one trained with data augmentation has a much smaller spread of errors.

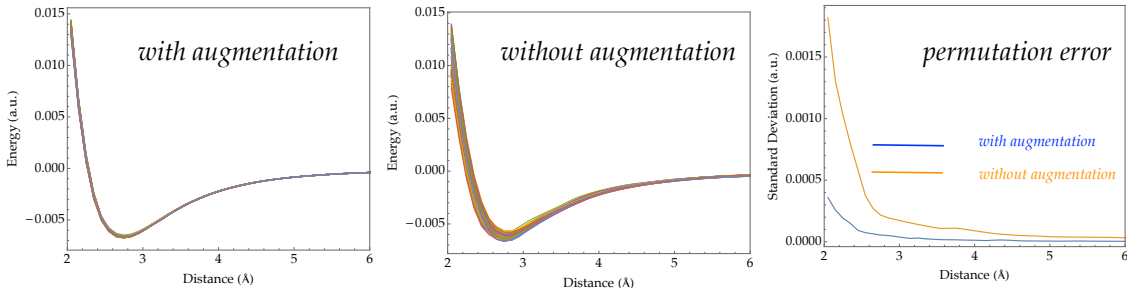


Figure 3: Left and middle panels: Change of the total two-body energy as one methanol is pulled away from the other two in a methanol trimer, calculated by the neural network trained with data augmentation (left) and without data augmentation (middle). Each of the possible 72 permutations is plotted on both panels. Right panel: Standard deviation of the 72 energies predicted by the neural network. One can see the neural network trained with data augmentation predicts a much more consistent energy for the different permuted Coulomb matrices.

Learning permutation invariance

The permutation invariance is learned by augmenting all the possible permutations for the samples into the training data set. For one-body cases, there are 6 possible permutations since the three hydrogen atoms on a methyl group are equivalent. The methanol dimer has two methyl groups and two interchangeable molecules, therefore it has 72 possible permutations. For the same reason, the methanol trimer has 1296 possible permutations, and it is difficult to include all of them. Therefore, we combine the chemically inert hydrogen atoms

on a methyl group into one imaginary atom by taking the average of the coordination of the three hydrogen atoms, which eliminates the permutations of hydrogen atoms on a methyl group and left 6 possible permutations caused by the interchange of methanol molecules in a methanol trimer.

The histogram of the two-body energy error of the the neural network that is trained with augmentation and without augmentation is shown in Figure 2. The test data set includes all the 72 possible permutations of the coulomb matrix of the original test data set. Error of the two-body energy is examined here since it has the most possible permutations of all of the many-body energy terms. One can see that the error of the neural network trained without augmentations is spread over the axis, while the error of the neural network trained with augmentation mostly populates in the region between -10^{-5} a.u. and 10^{-5} a.u.. The change of the total two-body energy, predicted by the neural network, when one methanol is pulled away from the other two methanols in a three methanol cluster, is shown in the left and middle panels of Figure 3. Each thin line in the two panels shows the two-body energy that is predicted by neural network based on one possible permutation of the coulomb matrix, which means there are 72 lines in each figure. The left panel of Figure 3 shows the standard deviation of the energies predicted by the neural network based on all the 72 possible coulomb matrix. One can see that, compared with the one trained without data augmentation, the neural network trained with data augmentation predicts a much more consistent energy for the 72 different permuted Coulomb matrices, which shows the neural network learns the permutation invariance from the augmented training data.

Molecular dynamic trajectory

Figure 4 shows the potential energy surface (PES) calculated by MP2-MBE and our NN-MBE. One can see that the two curves basically overlap with each other and the energy difference between MP2-MBE and NN-MBE is smaller than 10^{-3} a.u..

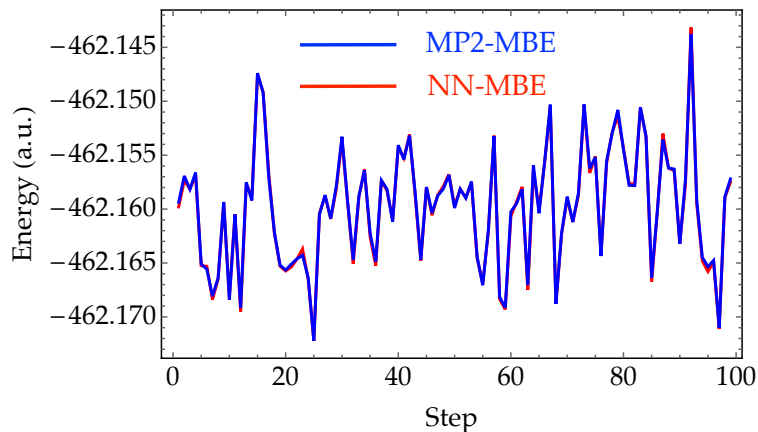


Figure 4: PES calculated by MP2-MBE (blue) and NN-MBE (red) of 4 methanol molecules along 100 steps of a molecular dynamic trajectory at 330 K. The NN-MBE predicts energies consistent with the MP2-MBE and the energy difference between MP2-MBE and NN-MBE is smaller than 10^{-3} a.u..

Timing

Figure 5 shows the total wall time comparison of NN-MBE, MP2-MBE and AMOEBA09. Since a cutoff of 10 Å is induced, both the NN-MBE and MP2-MBE will be near linear scaling at large cluster sizes. However, one can notice that NN-MBE has a speed up of more than two million relative to MP2-MBE, which enables us to use the NN-MBE to calculate the energy of large clusters of thousands of molecules in seconds with ab-initio level accuracy, which would take months for an MP2-MBE calculation. The AMOEBA09 calculation is done with the *TINKER* package. The total wall time of the NN-MBE is similar to AMOEBA09.

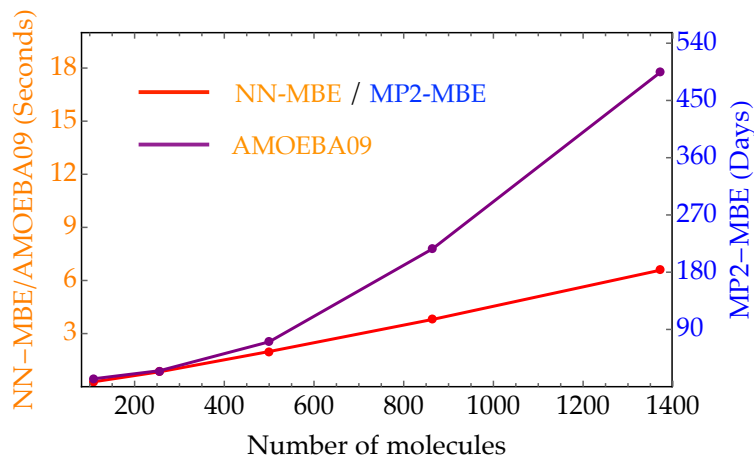


Figure 5: Total wall time for the NN-MBE (red curve, left orange y-axis), MP2-MBE (red, curve, right blue y-axis) AMOEBA09 (purple curve, left orange y-axis) to calculate the energies of methanol clusters of different size. One can see that NN-MBE has a more than two million times speed up over MP2-MBE.¹

Comparison with AMOEBA09

The PES predicted by the NN-MBE and AMOEBA09 when one methanol in a methanol trimer is pulled away from the other two is also compared in Figure 6. Both the NN-MBE and AMOEBA09 get the general shape of the PES and the minimum energy position correct, but the PES predicted by the NN-MBE is a better fit to the PES calculated using MP2, than the PES predicted by AMOEBA09.

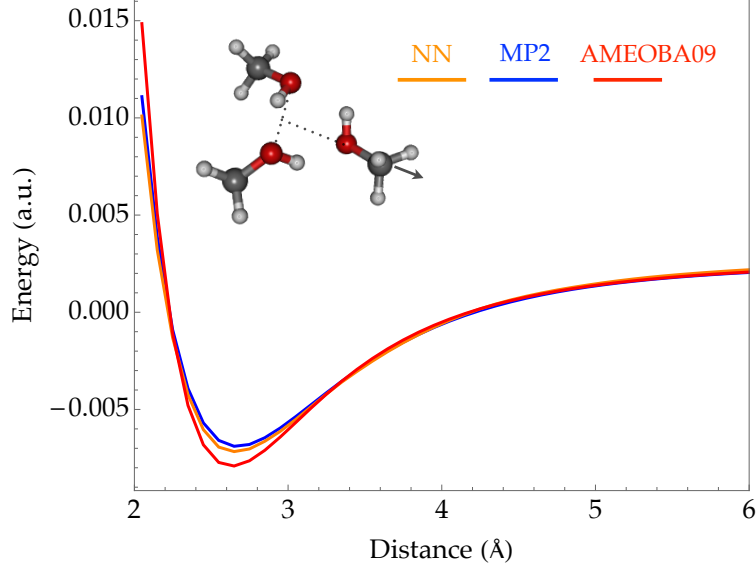


Figure 6: Change of the total energy when one methanol is pulled away from the other two in a methanol trimer, calculated by NN-MBE, MP2 and AMOEBA09. One can see that NN-MBE has better agreement with MP2 than AMOEBA09.

Neural network many-body expansion of dense helium

We built a NN-MBE model for a dense helium system with our code *Tensormol*. The average distance between two helium atoms in the system is 1\AA . In this scenario, the high order terms become significant and we calculated up to fourth order many-body terms. As one can see from Figure 7, our neural network predicts the many-body energy of the dense helium system accurately, including the fourth-body energy.

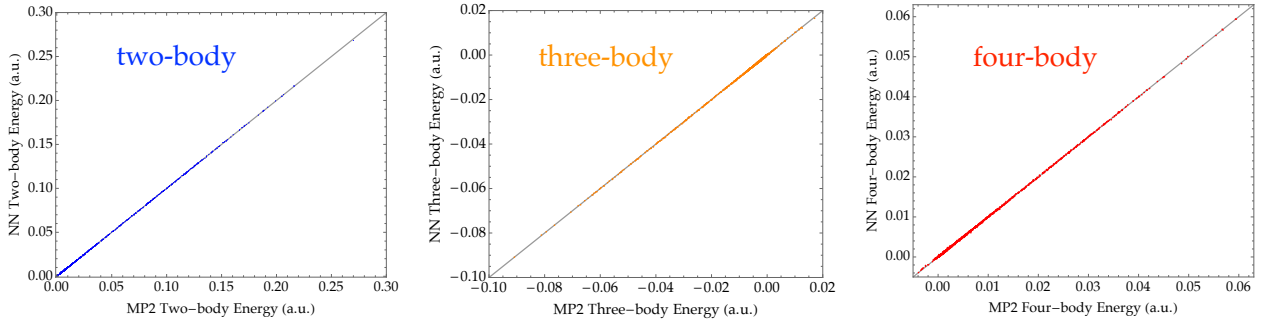


Figure 7: Left, middle and right panels show plots of the two-body, three-body, and four-body energies of a dense helium system. X-axis shows the energies calculated from MP2 and y-axis shows the energies predicted by our trained neural network.

Code

NN-MBE code is available in *tensormol*: https://github.com/jparkhill/TensorMol_MBE.git

Depth map code:

```
double abin = 0.143;
double reabin = 1/abin;
int xa, ya, za;
double x, y, z, dist;
double testpos[3];

double vdWC = 1.85/3;
double vdWH = 1.2/3;
double vdWO = 1.40/3;

int posmax = (vdWC*reabin);

for(int m=0; m<18;m++) {
    xa = xyz_[m*3]*reabin;
    ya = xyz_[m*3+1]*reabin;
    za = xyz_[m*3+2]*reabin;

    for(int j=-(posmax+4);j<(posmax+5);j++)
        for(int k=-(posmax+4);k<(posmax+5);k++)
            for(int l=-(posmax+4);l<(posmax+5);l++) {

                testpos[0] = (xa+j)*abin;
```



```

testpos[1] = (ya+k)*abin;
testpos[2] = (za+l)*abin;

x = testpos[0]-xa*abin;
y = testpos[1]-ya*abin;
z = testpos[2]-za*abin;

dist = (x*x)+(y*y)+(z*z);
dist = sqrt(dist);
if (deppl_[(xa+j)*width+(ya+k)] == 0) {
    if (idxlist_[m] == 1) {
        if (dist <= vdWC) {
            deppl_[(xa+j)*width+(ya+k)] = (za+l)*abin;
            break;
        }
    }
    if (idxlist_[m] == 2) {
        if (dist <= vdWO) {
            deppl_[(xa+j)*width+(ya+k)] = (za+l)*abin;
            break;
        }
    }
    if (idxlist_[m] == 0) {
        if (dist <= vdWH) {
            deppl_[(xa+j)*width+(ya+k)] = (za+l)*abin;
            break;
        }
    }
}
}

```

```

if (depl_[(xa+j)*width+(ya+k)] != 0) {

    if (idxlist_[m] == 1) {
        if (dist <= vdWC) {
            if ((za+l)*abin < depl_[(xa+j)*width+(ya+k)]) {
                depl_[(xa+j)*width+(ya+k)] = (za+l)*abin;
                break;
            }
        }
    }

    if (idxlist_[m] == 2) {
        if (dist <= vdWO) {
            if ((za+l)*abin < depl_[(xa+j)*width+(ya+k)]) {
                depl_[(xa+j)*width+(ya+k)] = (za+l)*abin;
                break;
            }
        }
    }

    if (idxlist_[m] == 0) {
        if (dist <= vdWH) {
            if ((za+l)*abin < depl_[(xa+j)*width+(ya+k)]) {
                depl_[(xa+j)*width+(ya+k)] = (za+l)*abin;
                break;
            }
        }
    }
}

}
}

```

References

- (1) Kavzoglu, T. Determining optimum structure for artificial neural networks. Proceedings of the 25th Annual Technical Conference and Exhibition of the Remote Sensing Society. 1999; pp 675–682.
- (2) Hastie, T.; Tibshirani, R.; Friedman, J.; Franklin, J. *Math. Intel.* **2005**, *27*, 83–85.

¹The NN-MBE calculations were done using one Tesla K80 GPU, MP2-MBE calculations were done with one 24-core CPU and AMOEBA09 calculation was performed on one CPU using *TINKER* package.

Data for Figure 3:

Coordinations(angstrom), Distance (angstrom), MP2 / NN two-body energies (a.u.) and three-body energies (a.u.) of all the 55 methanol clusters. Notice that the one-body energies of system do not change here:

```
C -1.702083  1.928529 -0.25332
O -0.60438  1.359481  0.435961
H -1.422001  2.934757 -0.537838
H -1.951775  1.372474 -1.154524
H -2.584355  1.984723  0.379279
H -0.831192  0.439469  0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164  0.654786
H -2.257564 -2.326338  0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H  0.313314 -1.155755  0.239809
C  2.368985 -0.318289  0.408733
O  1.291533  0.351088 -0.224173
H  2.689034 -1.114974 -0.250619
H  3.210193  0.349985  0.573211
H  2.07331 -0.751376  1.36117
H  0.95612  1.023414  0.395789
```

Distance: 2.04876

MP2: 2-body 0.0076835 3-body -0.0054756

NN: 2-body 0.0064667 3-body -0.0052691

```
C -1.702083  1.928529 -0.25332
O -0.60438  1.359481  0.435961
H -1.422001  2.934757 -0.537838
H -1.951775  1.372474 -1.154524
H -2.584355  1.984723  0.379279
H -0.831192  0.439469  0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164  0.654786
H -2.257564 -2.326338  0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H  0.313314 -1.155755  0.239809
C  2.460006 -0.300843  0.371172
O  1.382554  0.368534 -0.261734
H  2.780054 -1.097528 -0.28818
H  3.301214  0.367431  0.535649
H  2.16433 -0.73393  1.323608
H  1.047141  1.04086  0.358228
```

Distance: 2.14876

MP2: 2-body -0.0004082 3-body -0.0045875

NN: 2-body -0.0011725 3-body -0.0045222

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	2.551027	-0.283396	0.33361
O	1.473575	0.385981	-0.299296
H	2.871075	-1.080082	-0.325742
H	3.392234	0.384877	0.498088
H	2.255351	-0.716484	1.286047
H	1.138162	1.058307	0.320666

Distance: 2.24876

MP2: 2-body -0.0059418 3-body -0.0038343

NN: 2-body -0.0063150 3-body -0.0038919

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	2.642047	-0.26595	0.296049
O	1.564595	0.403427	-0.336857
H	2.962096	-1.062636	-0.363304
H	3.483255	0.402323	0.460526
H	2.346372	-0.699037	1.248485
H	1.229182	1.075753	0.283105

Distance: 2.34876

MP2: 2-body -0.0095971 3-body -0.0032032

NN: 2-body -0.0097868 3-body -0.0033568

C	-1.702083	1.928529	-0.25332
---	-----------	----------	----------

O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 2.733068 -0.248504 0.258487
O 1.655616 0.420873 -0.374419
H 3.053116 -1.045189 -0.400865
H 3.574276 0.419769 0.422965
H 2.437392 -0.681591 1.210924
H 1.320203 1.093199 0.245543

Distance: 2.44876

MP2: 2-body -0.0118948 3-body -0.0026795

NN: 2-body -0.0120199 3-body -0.0029173

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 2.824089 -0.231058 0.220926
O 1.746637 0.438319 -0.411981
H 3.144137 -1.027743 -0.438427
H 3.665296 0.437215 0.385403
H 2.528413 -0.664145 1.173362
H 1.411224 1.110645 0.207982

Distance: 2.54876

MP2: 2-body -0.0132270 3-body -0.0022476

NN: 2-body -0.0133019 3-body -0.0025343

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329

C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	2.915109	-0.213612	0.183364
O	1.837657	0.455765	-0.449542
H	3.235158	-1.010297	-0.475988
H	3.756317	0.454662	0.347842
H	2.619434	-0.646699	1.135801
H	1.502244	1.128091	0.17042

Distance: 2.64876

MP2: 2-body -0.0138851 3-body -0.0018927

NN: 2-body -0.0138940 3-body -0.0021737

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	3.00613	-0.196166	0.145802
O	1.928678	0.473211	-0.487104
H	3.326178	-0.992851	-0.51355
H	3.847338	0.472108	0.31028
H	2.710454	-0.629253	1.098239
H	1.593265	1.145537	0.132858

Distance: 2.74876

MP2: 2-body -0.0140826 3-body -0.0016016

NN: 2-body -0.0140507 3-body -0.0018805

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953

H 0.313314 -1.155755 0.239809
C 3.097151 -0.178719 0.108241
O 2.019699 0.490657 -0.524665
H 3.417199 -0.975405 -0.551111
H 3.938358 0.489554 0.272719
H 2.801475 -0.611807 1.060677
H 1.684286 1.162984 0.095297

Distance: 2.84876

MP2: 2-body -0.0139744 3-body -0.0013628

NN: 2-body -0.0139200 3-body -0.0016157

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.188171 -0.161273 0.070679
O 2.110719 0.508104 -0.562227
H 3.50822 -0.957959 -0.588673
H 4.029379 0.507 0.235157
H 2.892496 -0.59436 1.023116
H 1.775306 1.18043 0.057735

Distance: 2.94876

MP2: 2-body -0.0136716 3-body -0.0011668

NN: 2-body -0.0136295 3-body -0.0013972

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.279192 -0.143827 0.033118
O 2.20174 0.52555 -0.599788
H 3.59924 -0.940513 -0.626234
H 4.1204 0.524446 0.197595

H 2.983516 -0.576914 0.985554
H 1.866327 1.197876 0.020174
Distance: 3.04876
MP2: 2-body -0.0132526 3-body -0.0010053
NN: 2-body -0.0131992 3-body -0.0012214

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.370213 -0.126381 -0.004444
O 2.292761 0.542996 -0.63735
H 3.690261 -0.923066 -0.663796
H 4.21142 0.541892 0.160034
H 3.074537 -0.559468 0.947993
H 1.957348 1.215322 -0.017388
Distance: 3.14876
MP2: 2-body -0.0127722 3-body -0.0008720
NN: 2-body -0.0126986 3-body -0.0010688

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.461233 -0.108935 -0.042005
O 2.383781 0.560442 -0.674911
H 3.781282 -0.90562 -0.701358
H 4.302441 0.559339 0.122472
H 3.165558 -0.542022 0.910431
H 2.048368 1.232768 -0.054949
Distance: 3.24876
MP2: 2-body -0.0122680 3-body -0.0007613
NN: 2-body -0.0121684 3-body -0.0009448

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	3.552254	-0.091489	-0.079567
O	2.474802	0.577888	-0.712473
H	3.872302	-0.888174	-0.738919
H	4.393462	0.576785	0.084911
H	3.256578	-0.524576	0.87287
H	2.139389	1.250214	-0.092511

Distance: 3.34876

MP2: 2-body -0.0117651 3-body -0.0006688

NN: 2-body -0.0116587 3-body -0.0008372

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	3.643275	-0.074043	-0.117128
O	2.565823	0.595334	-0.750035
H	3.963323	-0.870728	-0.776481
H	4.484482	0.594231	0.047349
H	3.347599	-0.50713	0.835308
H	2.23041	1.26766	-0.130072

Distance: 3.44876

MP2: 2-body -0.0112798 3-body -0.0005909

NN: 2-body -0.0111952 3-body -0.0007454

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524

H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.734295 -0.056596 -0.15469
O 2.656843 0.612781 -0.787596
H 4.054344 -0.853282 -0.814042
H 4.575503 0.611677 0.009788
H 3.43862 -0.489684 0.797747
H 2.32143 1.285107 -0.167634

Distance: 3.54876

MP2: 2-body -0.0108220 3-body -0.0005248

NN: 2-body -0.0107482 3-body -0.0006665

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.825316 -0.03915 -0.192252
O 2.747864 0.630227 -0.825158
H 4.145364 -0.835836 -0.851604
H 4.666524 0.629123 -0.027774
H 3.52964 -0.472237 0.760185
H 2.412451 1.302553 -0.205196

Distance: 3.64876

MP2: 2-body -0.0103970 3-body -0.0004682

NN: 2-body -0.0103251 3-body -0.0005973

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474

H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 3.916337 -0.021704 -0.229813
O 2.838885 0.647673 -0.862719
H 4.236385 -0.818389 -0.889165
H 4.757544 0.646569 -0.065335
H 3.620661 -0.454791 0.722623
H 2.503472 1.319999 -0.242757

Distance: 3.74876

MP2: 2-body -0.0100068 3-body -0.0004193

NN: 2-body -0.0099316 3-body -0.0005369

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.007357 -0.004258 -0.267375
O 2.929905 0.665119 -0.900281
H 4.327406 -0.800943 -0.926727
H 4.848565 0.664016 -0.102897
H 3.711682 -0.437345 0.685062
H 2.594492 1.337445 -0.280319

Distance: 3.84876

MP2: 2-body -0.0096516 3-body -0.0003767

NN: 2-body -0.0095715 3-body -0.0004820

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.098378 0.013188 -0.304936
O 3.020926 0.682565 -0.937842

H 4.418426 -0.783497 -0.964288
H 4.939586 0.681462 -0.140459
H 3.802702 -0.419899 0.6475
H 2.685513 1.354891 -0.31788

Distance: 3.94876

MP2: 2-body -0.0093299 3-body -0.0003393

NN: 2-body -0.0092371 3-body -0.0004332

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.189399 0.030634 -0.342498
O 3.111947 0.700011 -0.975404
H 4.509447 -0.766051 -1.00185
H 5.030606 0.698908 -0.17802
H 3.893723 -0.402453 0.609939
H 2.776534 1.372337 -0.355442

Distance: 4.04876

MP2: 2-body -0.0090399 3-body -0.0003062

NN: 2-body -0.0089296 3-body -0.0003920

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.280419 0.048081 -0.380059
O 3.202967 0.717457 -1.012965
H 4.600468 -0.748605 -1.039412
H 5.121627 0.716354 -0.215582
H 3.984744 -0.385007 0.572377
H 2.867554 1.389784 -0.393003

Distance: 4.14876

MP2: 2-body -0.0087790 3-body -0.0002768
NN: 2-body -0.0086580 3-body -0.0003529

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.37144 0.065527 -0.417621
O 3.293988 0.734904 -1.050527
H 4.691488 -0.731159 -1.076973
H 5.212648 0.7338 -0.253143
H 4.075764 -0.36756 0.534816
H 2.958575 1.40723 -0.430565

Distance: 4.24876

MP2: 2-body -0.0085447 3-body -0.0002503
NN: 2-body -0.0084114 3-body -0.0003151

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.462461 0.082973 -0.455182
O 3.385009 0.75235 -1.088089
H 4.782509 -0.713713 -1.114535
H 5.303668 0.751246 -0.290705
H 4.166785 -0.350114 0.497254
H 3.049596 1.424676 -0.468126

Distance: 4.34876

MP2: 2-body -0.0083346 3-body -0.0002265
NN: 2-body -0.0081960 3-body -0.0002839

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961

H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.553481 0.100419 -0.492744
O 3.476029 0.769796 -1.12565
H 4.87353 -0.696266 -1.152096
H 5.394689 0.768692 -0.328266
H 4.257806 -0.332668 0.459693
H 3.140616 1.442122 -0.505688

Distance: 4.44876

MP2: 2-body -0.0081462 3-body -0.0002049

NN: 2-body -0.0080063 3-body -0.0002598

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.644502 0.117865 -0.530305
O 3.56705 0.787242 -1.163212
H 4.96455 -0.67882 -1.189658
H 5.48571 0.786139 -0.365828
H 4.348826 -0.315222 0.422131
H 3.231637 1.459568 -0.54325

Distance: 4.54876

MP2: 2-body -0.0079773 3-body -0.0001855

NN: 2-body -0.0078392 3-body -0.0002369

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655

O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.735523 0.135311 -0.567867
O 3.658071 0.804688 -1.200773
H 5.055571 -0.661374 -1.227219
H 5.57673 0.803585 -0.403389
H 4.439847 -0.297776 0.384569
H 3.322658 1.477014 -0.580811

Distance: 4.64876

MP2: 2-body -0.0078258 3-body -0.0001679

NN: 2-body -0.0076920 3-body -0.0002160

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 4.826543 0.152758 -0.605429
O 3.749091 0.822134 -1.238335
H 5.146592 -0.643928 -1.264781
H 5.667751 0.821031 -0.440951
H 4.530868 -0.28033 0.347008
H 3.413678 1.494461 -0.618373

Distance: 4.74876

MP2: 2-body -0.0076900 3-body -0.0001521

NN: 2-body -0.0075605 3-body -0.0001966

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809

C 4.917564 0.170204 -0.64299
O 3.840112 0.839581 -1.275896
H 5.237612 -0.626482 -1.302342
H 5.758772 0.838477 -0.478513
H 4.621888 -0.262884 0.309446
H 3.504699 1.511907 -0.655934

Distance: 4.84876

MP2: 2-body -0.0075681 3-body -0.0001380

NN: 2-body -0.0074397 3-body -0.0001818

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.008585 0.18765 -0.680552
O 3.931133 0.857027 -1.313458
H 5.328633 -0.609036 -1.339904
H 5.849792 0.855923 -0.516074
H 4.712909 -0.245437 0.271885
H 3.59572 1.529353 -0.693496

Distance: 4.94876

MP2: 2-body -0.0074585 3-body -0.0001254

NN: 2-body -0.0073299 3-body -0.0001682

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.099605 0.205096 -0.718113
O 4.022153 0.874473 -1.351019
H 5.419654 -0.591589 -1.377466
H 5.940813 0.873369 -0.553636
H 4.80393 -0.227991 0.234323

H 3.68674 1.546799 -0.731057
Distance: 5.04876
MP2: 2-body -0.0073598 3-body -0.0001142
NN: 2-body -0.0072279 3-body -0.0001555

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.190626 0.222542 -0.755675
O 4.113174 0.891919 -1.388581
H 5.510674 -0.574143 -1.415027
H 6.031834 0.890816 -0.591197
H 4.89495 -0.210545 0.196762
H 3.777761 1.564245 -0.768619

Distance: 5.14876
MP2: 2-body -0.0072709 3-body -0.0001044
NN: 2-body -0.0071369 3-body -0.0001436

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.281647 0.239988 -0.793236
O 4.204195 0.909365 -1.426143
H 5.601695 -0.556697 -1.452589
H 6.122854 0.908262 -0.628759
H 4.985971 -0.193099 0.1592
H 3.868782 1.581691 -0.80618

Distance: 5.24876
MP2: 2-body -0.0071905 3-body -0.0000957
NN: 2-body -0.0070540 3-body -0.0001327

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.372667 0.257434 -0.830798
O 4.295215 0.926811 -1.463704
H 5.692715 -0.539251 -1.49015
H 6.213875 0.925708 -0.66632
H 5.076992 -0.175653 0.121639
H 3.959802 1.599137 -0.843742

Distance: 5.34876

MP2: 2-body -0.0071178 3-body -0.0000880

NN: 2-body -0.0069793 3-body -0.0001222

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.463688 0.274881 -0.868359
O 4.386236 0.944257 -1.501266
H 5.783736 -0.521805 -1.527712
H 6.304896 0.943154 -0.703882
H 5.168012 -0.158207 0.084077
H 4.050823 1.616584 -0.881304

Distance: 5.44876

MP2: 2-body -0.0070519 3-body -0.0000812

NN: 2-body -0.0069137 3-body -0.0001127

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279

H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.554709 0.292327 -0.905921
O 4.477257 0.961704 -1.538827
H 5.874757 -0.504359 -1.565273
H 6.395916 0.9606 -0.741443
H 5.259033 -0.14076 0.046515
H 4.141844 1.63403 -0.918865

Distance: 5.54876

MP2: 2-body -0.0069920 3-body -0.0000753

NN: 2-body -0.0068545 3-body -0.0001037

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.645729 0.309773 -0.943483
O 4.568277 0.97915 -1.576389
H 5.965777 -0.486912 -1.602835
H 6.486937 0.978046 -0.779005
H 5.350054 -0.123314 0.008954
H 4.232864 1.651476 -0.956427

Distance: 5.64876

MP2: 2-body -0.0069374 3-body -0.0000700

NN: 2-body -0.0068013 3-body -0.0000947

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503

H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.73675 0.327219 -0.981044
O 4.659298 0.996596 -1.61395
H 6.056798 -0.469466 -1.640396
H 6.577958 0.995492 -0.816567
H 5.441074 -0.105868 -0.028608
H 4.323885 1.668922 -0.993988

Distance: 5.74876

MP2: 2-body -0.0068875 3-body -0.0000653

NN: 2-body -0.0067520 3-body -0.0000860

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.827771 0.344665 -1.018606
O 4.750319 1.014042 -1.651512
H 6.147819 -0.45202 -1.677958
H 6.668978 1.012939 -0.854128
H 5.532095 -0.088422 -0.066169
H 4.414906 1.686368 -1.03155

Distance: 5.84876

MP2: 2-body -0.0068420 3-body -0.0000611

NN: 2-body -0.0067062 3-body -0.0000777

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 5.918791 0.362111 -1.056167
O 4.841339 1.031488 -1.689073
H 6.238839 -0.434574 -1.71552

H 6.759999 1.030385 -0.89169
H 5.623116 -0.070976 -0.103731
H 4.505926 1.703814 -1.069111
Distance: 5.94876
MP2: 2-body -0.0068002 3-body -0.0000573
NN: 2-body -0.0066640 3-body -0.0000708

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.009812 0.379558 -1.093729
O 4.93236 1.048934 -1.726635
H 6.32986 -0.417128 -1.753081
H 6.85102 1.047831 -0.929251
H 5.714136 -0.05353 -0.141292
H 4.596947 1.721261 -1.106673
Distance: 6.04876
MP2: 2-body -0.0067618 3-body -0.0000539
NN: 2-body -0.0066254 3-body -0.0000647

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.100833 0.397004 -1.13129
O 5.023381 1.066381 -1.764197
H 6.420881 -0.399682 -1.790643
H 6.94204 1.065277 -0.966813
H 5.805157 -0.036084 -0.178854
H 4.687968 1.738707 -1.144234
Distance: 6.14876
MP2: 2-body -0.0067265 3-body -0.0000508

NN: 2-body -0.0065902 3-body -0.0000594

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	6.191853	0.41445	-1.168852
O	5.114401	1.083827	-1.801758
H	6.511901	-0.382236	-1.828204
H	7.033061	1.082723	-1.004374
H	5.896178	-0.018637	-0.216415
H	4.778988	1.756153	-1.181796

Distance: 6.24876

MP2: 2-body -0.0066939 3-body -0.0000479

NN: 2-body -0.0065572 3-body -0.0000542

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	6.282874	0.431896	-1.206413
O	5.205422	1.101273	-1.83932
H	6.602922	-0.364789	-1.865766
H	7.124082	1.100169	-1.041936
H	5.987198	-0.001191	-0.253977
H	4.870009	1.773599	-1.219358

Distance: 6.34876

MP2: 2-body -0.0066639 3-body -0.0000453

NN: 2-body -0.0065261 3-body -0.0000493

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838

H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.373895 0.449342 -1.243975
O 5.296443 1.118719 -1.876881
H 6.693943 -0.347343 -1.903327
H 7.215102 1.117616 -1.079497
H 6.078219 0.016255 -0.291539
H 4.96103 1.791045 -1.256919

Distance: 6.44876

MP2: 2-body -0.0066361 3-body -0.0000429

NN: 2-body -0.0064975 3-body -0.0000449

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.464915 0.466788 -1.281537
O 5.387463 1.136165 -1.914443
H 6.784963 -0.329897 -1.940889
H 7.306123 1.135062 -1.117059
H 6.16924 0.033701 -0.3291
H 5.05205 1.808491 -1.294481

Distance: 6.54876

MP2: 2-body -0.0066104 3-body -0.0000407

NN: 2-body -0.0064712 3-body -0.0000408

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786

H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.555936 0.484234 -1.319098
O 5.478484 1.153611 -1.952004
H 6.875984 -0.312451 -1.97845
H 7.397144 1.152508 -1.154621
H 6.26026 0.051147 -0.366662
H 5.143071 1.825937 -1.332042

Distance: 6.64876

MP2: 2-body -0.0065865 3-body -0.0000386

NN: 2-body -0.0064468 3-body -0.0000369

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.646957 0.501681 -1.35666
O 5.569505 1.171058 -1.989566
H 6.967005 -0.295005 -2.016012
H 7.488164 1.169954 -1.192182
H 6.351281 0.068593 -0.404223
H 5.234092 1.843384 -1.369604

Distance: 6.74876

MP2: 2-body -0.0065643 3-body -0.0000366

NN: 2-body -0.0064238 3-body -0.0000336

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.737977 0.519127 -1.394221

O 5.660525 1.188504 -2.027127
H 7.058025 -0.277559 -2.053574
H 7.579185 1.1874 -1.229744
H 6.442302 0.08604 -0.441785
H 5.325112 1.86083 -1.407165

Distance: 6.84876

MP2: 2-body -0.0065437 3-body -0.0000348

NN: 2-body -0.0064025 3-body -0.0000310

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.828998 0.536573 -1.431783
O 5.751546 1.20595 -2.064689
H 7.149046 -0.260112 -2.091135
H 7.670206 1.204846 -1.267305
H 6.533322 0.103486 -0.479346
H 5.416133 1.878276 -1.444727

Distance: 6.94876

MP2: 2-body -0.0065245 3-body -0.0000331

NN: 2-body -0.0063831 3-body -0.0000287

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 6.920019 0.554019 -1.469344
O 5.842567 1.223396 -2.102251
H 7.240067 -0.242666 -2.128697
H 7.761226 1.222292 -1.304867
H 6.624343 0.120932 -0.516908
H 5.507154 1.895722 -1.482288

Distance: 7.04876

MP2: 2-body -0.0065067 3-body -0.0000316

NN: 2-body -0.0063643 3-body -0.0000267

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	7.011039	0.571465	-1.506906
O	5.933587	1.240842	-2.139812
H	7.331087	-0.22522	-2.166258
H	7.852247	1.239739	-1.342428
H	6.715364	0.138378	-0.554469
H	5.598174	1.913168	-1.51985

Distance: 7.14876

MP2: 2-body -0.0064900 3-body -0.0000301

NN: 2-body -0.0063471 3-body -0.0000250

C	-1.702083	1.928529	-0.25332
O	-0.60438	1.359481	0.435961
H	-1.422001	2.934757	-0.537838
H	-1.951775	1.372474	-1.154524
H	-2.584355	1.984723	0.379279
H	-0.831192	0.439469	0.664329
C	-1.275358	-2.156977	-0.268655
O	-0.542144	-1.372164	0.654786
H	-2.257564	-2.326338	0.154474
H	-1.391246	-1.655864	-1.227503
H	-0.803534	-3.121733	-0.435953
H	0.313314	-1.155755	0.239809
C	7.10206	0.588911	-1.544467
O	6.024608	1.258288	-2.177374
H	7.422108	-0.207774	-2.20382
H	7.943268	1.257185	-1.37999
H	6.806384	0.155824	-0.592031
H	5.689195	1.930614	-1.557412

Distance: 7.24876

MP2: 2-body -0.0064744 3-body -0.0000287

NN: 2-body -0.0063310 3-body -0.0000234

C	-1.702083	1.928529	-0.25332
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O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 7.193081 0.606358 -1.582029
O 6.115629 1.275734 -2.214935
H 7.513129 -0.190328 -2.241381
H 8.034288 1.274631 -1.417551
H 6.897405 0.17327 -0.629593
H 5.780216 1.948061 -1.594973

Distance: 7.34876

MP2: 2-body -0.0064598 3-body -0.0000274

NN: 2-body -0.0063163 3-body -0.0000219

C -1.702083 1.928529 -0.25332
O -0.60438 1.359481 0.435961
H -1.422001 2.934757 -0.537838
H -1.951775 1.372474 -1.154524
H -2.584355 1.984723 0.379279
H -0.831192 0.439469 0.664329
C -1.275358 -2.156977 -0.268655
O -0.542144 -1.372164 0.654786
H -2.257564 -2.326338 0.154474
H -1.391246 -1.655864 -1.227503
H -0.803534 -3.121733 -0.435953
H 0.313314 -1.155755 0.239809
C 7.284101 0.623804 -1.619591
O 6.206649 1.293181 -2.252497
H 7.604149 -0.172882 -2.278943
H 8.125309 1.292077 -1.455113
H 6.988426 0.190716 -0.667154
H 5.871236 1.965507 -1.632535

Distance: 7.44876

MP2: 2-body -0.0064461 3-body -0.0000261

NN: 2-body -0.0063023 3-body -0.0000206

Data for Figure 4:

Coordinations(angstrom), relative MP2 / MP2-MBE / NN-MBE energies (a.u) of the 5 methanol clusters that consist of 20 methanol molecule. The relative energies are calculated as: *Energy of the cluster – Mean (Energy of the Five Clusters)*.

Cluster 1:

C	0.87795	-0.23893	1.03079
O	0.0	0.0	0.0
H	0.96587	0.71823	1.574
H	0.51217	-0.96426	1.73689
H	1.83718	-0.60676	0.66456
H	-0.70026	-0.62915	0.08934
C	0.06442	0.06828	-4.1723
O	-0.06035	0.56475	-2.81895
H	-0.45937	-0.83062	-4.26167
H	-0.22157	0.82343	-4.88087
H	1.08328	-0.05448	-4.38688
H	0.70797	0.36886	-2.2515
C	3.74316	0.71087	-2.12348
O	2.46367	0.91143	-1.54141
H	3.81779	1.34702	-2.96013
H	4.52249	0.93691	-1.41818
H	3.91345	-0.32039	-2.44765
H	2.59184	1.52422	-0.81681
C	-1.65305	-2.74377	0.92907
O	-2.40288	-1.52942	1.20564
H	-2.23744	-3.58761	1.18255
H	-1.25423	-2.74311	-0.12878
H	-0.8278	-2.71281	1.6162
H	-3.30698	-1.72491	1.47573
C	-0.35287	3.63661	-2.29379
O	0.42434	3.18557	-1.22194
H	-0.16445	4.73324	-2.45022
H	-0.06745	3.07005	-3.21746
H	-1.37221	3.48393	-2.09897
H	0.46382	2.20641	-1.29442
C	2.12687	-5.01135	0.1177
O	1.61028	-3.65187	-0.052
H	3.18811	-4.94999	0.20772
H	1.71363	-5.49896	0.98146
H	1.85357	-5.60852	-0.72304
H	1.97956	-3.22991	0.72906

C	4.59747	2.71169	0.84951
O	3.27456	2.3066	0.51753
H	4.92955	3.53454	0.24336
H	4.55988	2.92584	1.96368
H	5.24712	1.84856	0.73763
H	2.64408	2.79221	1.03863
C	3.64112	-3.74747	3.18137
O	3.35886	-2.83115	2.1214
H	2.97751	-3.535	4.06722
H	3.4334	-4.74023	2.73836
H	4.68658	-3.6351	3.40105
H	4.09135	-2.85273	1.5141
C	2.18038	3.06208	3.96642
O	1.77366	3.75697	2.8002
H	1.95663	3.60461	4.86012
H	1.69124	2.0908	4.01213
H	3.23277	2.89807	3.88316
H	0.89853	4.09828	2.99334
C	-1.13055	2.51711	2.53616
O	-1.0678	3.68315	3.32112
H	-0.38158	2.55847	1.77654
H	-0.99357	1.63689	3.13392
H	-2.14	2.43249	2.14582
H	-1.59032	3.54886	4.12394
C	-4.01671	-0.1134	-1.57191
O	-5.34865	-0.18487	-1.04645
H	-3.58784	0.91097	-1.54296
H	-3.3831	-0.69612	-0.97093
H	-4.00308	-0.54562	-2.60872
H	-5.94109	-0.48059	-1.75193
C	-4.83859	2.40755	1.83096
O	-4.88485	2.45165	0.38867
H	-4.38912	1.55499	2.16839
H	-4.29217	3.26154	2.18968
H	-5.80945	2.54295	2.27999
H	-5.25571	1.58858	0.05233
C	5.56734	-4.21736	-1.78216
O	4.55985	-3.5742	-1.04349
H	5.33424	-4.1616	-2.85981
H	6.50686	-3.80251	-1.63918
H	5.57481	-5.26052	-1.50495
H	3.98028	-3.09771	-1.68522
C	-6.81166	-0.88483	2.08686
O	-5.53251	-1.35891	2.24354
H	-7.25582	-1.29515	1.18648
H	-7.50596	-1.06673	2.97712
H	-6.76939	0.18756	1.89345
H	-5.06775	-0.88621	2.96671
C	1.27571	-3.67312	-3.66262

O	0.4911	-3.86406	-4.82053
H	2.3322	-3.48045	-3.87518
H	0.91973	-2.75942	-3.1388
H	1.19258	-4.53421	-3.01336
H	0.71858	-4.77263	-5.13018
C	-4.45456	-3.80205	4.07156
O	-3.23254	-4.38856	3.54974
H	-5.23569	-3.85019	3.29487
H	-4.7987	-4.40263	4.93148
H	-4.32213	-2.76367	4.40718
H	-2.52221	-4.27823	4.1629
C	4.79628	-2.43774	-5.5372
O	4.39395	-1.42184	-4.58371
H	5.75423	-2.9175	-5.30194
H	4.05672	-3.20395	-5.61193
H	4.91111	-2.04224	-6.59227
H	4.96533	-0.66967	-4.71322
C	2.70374	3.06249	-4.97228
O	1.48364	2.91588	-5.64069
H	3.32506	2.23489	-5.19224
H	3.14857	3.96453	-5.27959
H	2.47881	2.99289	-3.8675
H	1.66526	2.9571	-6.5661
C	1.05975	-1.06818	6.12096
O	-0.10263	-1.82536	6.26336
H	1.10695	-0.38772	6.92973
H	1.90808	-1.70204	6.13543
H	0.97811	-0.53493	5.19361
H	-0.79842	-1.24448	6.5321
C	2.95969	5.57264	-1.05781
O	2.6582	6.27521	0.22395
H	3.55468	4.68447	-0.8468
H	2.04146	5.23085	-1.57475
H	3.45886	6.23779	-1.72474
H	2.6032	5.67178	0.97515

MP2: -2311.00235
 MP2-MBE: -2310.93744
 MP2-NN: -2310.93545

Cluster 2:

C	-1.10074	-0.68898	0.29082
O	0.0	0.0	0.0
H	-0.92164	-1.78574	0.38104
H	-1.53782	-0.32823	1.21678
H	-1.84459	-0.62452	-0.51254

H	0.07938	0.32993	-0.9572
C	1.23804	0.45369	-2.90404
O	0.11192	1.29085	-2.79603
H	1.52913	0.49481	-3.9065
H	1.96891	1.03058	-2.35721
H	1.00442	-0.51965	-2.55018
H	0.45514	2.21011	-2.55833
C	1.07232	0.10038	3.57103
O	0.60738	1.32524	3.02857
H	1.48362	0.28069	4.56337
H	0.21375	-0.52619	3.65339
H	1.89926	-0.33761	2.90227
H	0.00715	1.10352	2.24369
C	-3.32626	2.69705	2.14699
O	-2.28658	2.26908	2.98672
H	-3.728	1.88348	1.60038
H	-4.13928	3.12202	2.74459
H	-3.00787	3.45914	1.52105
H	-2.26719	2.71794	3.89051
C	1.91389	3.34608	-0.3561
O	1.54776	4.27049	-1.41013
H	0.99622	3.05647	0.26237
H	2.33912	2.42277	-0.8276
H	2.67976	3.73859	0.36998
H	1.39573	5.12757	-1.01688
C	-0.97167	5.25054	2.89065
O	-0.20106	4.54827	1.93448
H	-0.38348	5.53247	3.78765
H	-1.36469	6.20718	2.43822
H	-1.87763	4.61867	3.06542
H	0.12005	3.7466	2.35948
C	-3.91008	0.24274	-2.35388
O	-4.43983	1.40935	-1.84039
H	-4.26812	-0.64992	-1.80846
H	-4.18099	0.20547	-3.38977
H	-2.87193	0.34671	-2.29077
H	-4.51646	1.98031	-2.60341
C	3.98734	3.15245	3.63796
O	2.89219	3.19684	2.78182
H	4.85225	2.95991	3.00258
H	4.08352	4.05961	4.20113
H	3.78917	2.31113	4.30166
H	2.2675	2.49812	3.10905
C	3.41546	-1.57057	-1.05541
O	4.62888	-1.73279	-1.56421
H	3.52372	-1.92748	-0.00192
H	3.13857	-0.5043	-1.05321
H	2.69649	-2.20576	-1.5498
H	5.00771	-2.45466	-0.9866

C	-1.00823	-3.00751	-4.00972
O	-2.09795	-2.11934	-4.26273
H	-0.00491	-2.53729	-4.26006
H	-0.92249	-3.3326	-2.91235
H	-1.1125	-3.87715	-4.65697
H	-2.88247	-2.57756	-3.89259
C	-2.032	6.02863	-0.71354
O	-2.24629	4.66297	-0.67806
H	-1.54659	6.37631	0.18246
H	-1.36497	6.28193	-1.57442
H	-3.04215	6.51116	-0.72653
H	-1.37674	4.20478	-0.75367
C	-2.68823	-1.47448	3.62715
O	-2.84379	-0.48385	4.62765
H	-3.32836	-1.22773	2.75991
H	-1.65514	-1.56939	3.2699
H	-2.96033	-2.47323	4.11701
H	-2.81687	0.41978	4.25721
C	2.76534	-2.84797	-5.38976
O	2.67037	-1.8983	-4.39235
H	3.0189	-2.3676	-6.36874
H	3.47468	-3.57815	-5.10692
H	1.81084	-3.38339	-5.52932
H	3.56547	-1.83721	-4.07318
C	-0.77622	-4.49497	4.31793
O	-0.36876	-3.24019	4.58647
H	-0.59901	-4.70624	3.26431
H	-0.15173	-5.21174	4.90488
H	-1.85278	-4.61143	4.55675
H	0.57256	-3.31397	4.84359
C	-4.18822	-4.02898	-0.54663
O	-3.91375	-3.62126	-1.84497
H	-3.56068	-4.89479	-0.24836
H	-4.04861	-3.21638	0.09937
H	-5.22551	-4.31632	-0.51263
H	-4.66793	-3.77583	-2.3791
C	3.40429	-5.84361	-2.45368
O	1.97226	-5.45035	-2.35088
H	3.51542	-6.93676	-2.46875
H	3.80621	-5.44741	-3.37201
H	4.08547	-5.45425	-1.691
H	1.48863	-6.26025	-2.34702
C	1.82942	7.35765	0.46912
O	0.96588	6.2971	0.055
H	1.34007	8.00792	1.22985
H	2.7295	6.87847	0.84554
H	2.08215	7.96547	-0.36438
H	0.68084	5.80523	0.89095
C	4.57973	-4.62096	1.81972

O	3.324	-5.22471	1.85717
H	5.30091	-5.29795	1.47129
H	4.60341	-3.66337	1.34835
H	4.83651	-4.37689	2.89777
H	3.2028	-5.56813	2.72615
C	0.64956	-5.42906	0.66014
O	0.35552	-6.81914	0.82476
H	1.5742	-5.34483	0.1187
H	-0.0728	-4.88298	0.03482
H	0.8808	-5.00006	1.56231
H	0.92998	-7.13285	1.52124
C	4.79727	3.1211	-3.79631
O	5.14486	3.89778	-2.62299
H	4.39538	2.1881	-3.49348
H	4.14971	3.70824	-4.40072
H	5.71744	2.8967	-4.38361
H	6.1027	3.9977	-2.63314

MP2: -2310.91947
 MP2-MBE: -2310.86004
 MP2-NN: -2310.85729

Cluster 3:

C	-0.0091	-1.22295	0.80545
O	0.0	0.0	0.0
H	-0.95375	-1.65957	0.70552
H	0.71437	-1.93857	0.42668
H	0.10144	-0.94047	1.78688
H	-0.9234	0.36802	-0.0341
C	-2.27835	2.95621	-0.28364
O	-2.47976	1.59256	-0.5035
H	-1.26315	3.06556	0.09519
H	-2.46936	3.63803	-1.17117
H	-2.91987	3.27961	0.50489
H	-2.85007	1.51381	-1.41053
C	2.93261	1.2695	1.2353
O	3.57721	1.4112	-0.00974
H	3.48585	1.76996	2.02795
H	1.8984	1.59963	1.17248
H	2.90524	0.27627	1.49151
H	3.5224	2.32355	-0.30472
C	4.54367	-1.68454	-0.21445
O	4.11498	-0.72771	-1.20887
H	3.83251	-1.77111	0.58213
H	4.68743	-2.65208	-0.7726
H	5.44278	-1.32874	0.20794

H	4.15906	0.13327	-0.80981
C	0.82914	-1.93661	-2.69079
O	1.17707	-1.95393	-3.99267
H	0.68055	-2.92313	-2.34558
H	1.59742	-1.44539	-2.06759
H	-0.15618	-1.57971	-2.43332
H	1.25914	-1.02366	-4.27401
C	0.84889	2.29546	-1.96977
O	1.30004	3.52731	-2.66166
H	-0.21972	2.02477	-2.19752
H	1.47596	1.41474	-2.33135
H	0.94273	2.34978	-0.82318
H	0.48479	4.05562	-2.70124
C	-2.16342	-3.06724	3.72919
O	-0.81265	-3.21447	3.26849
H	-2.56293	-2.04152	3.4901
H	-2.77357	-3.77319	3.16591
H	-2.2228	-3.22058	4.83347
H	-0.26438	-2.7371	3.86297
C	-4.87106	-0.44777	0.76806
O	-4.55299	0.52183	1.77866
H	-5.73913	-0.14625	0.21516
H	-3.99348	-0.5815	0.05676
H	-5.08683	-1.40695	1.30932
H	-5.09914	1.30683	1.69298
C	-0.8723	0.57879	4.02403
O	-0.7954	-0.53366	4.83053
H	-0.24217	1.33503	4.42466
H	-0.58332	0.29012	3.02657
H	-1.96554	0.97697	4.00653
H	0.13336	-0.60731	5.10276
C	-4.71514	0.40438	-2.68792
O	-3.91999	1.5733	-2.81212
H	-4.32474	-0.40623	-3.2647
H	-4.70513	0.16412	-1.627
H	-5.76801	0.5904	-3.06935
H	-4.29793	2.34496	-3.2973
C	-1.52945	-4.21208	-1.69126
O	-0.5406	-5.12842	-1.48998
H	-1.42889	-3.53951	-0.83823
H	-1.30124	-3.69102	-2.61339
H	-2.51441	-4.69987	-1.73655
H	-0.66979	-5.8056	-2.18527
C	2.73297	-2.52335	4.14088
O	2.26039	-1.47475	4.956
H	3.77026	-2.27344	3.80986
H	2.69424	-3.42331	4.6511
H	2.05359	-2.64399	3.247
H	3.05098	-1.05381	5.29103

C	1.38618	-7.02899	0.90045
O	1.14229	-5.61741	0.83548
H	0.63803	-7.51101	1.50264
H	1.35168	-7.4886	-0.08077
H	2.34714	-7.22823	1.33384
H	0.61245	-5.32757	0.02652
C	5.47274	0.43454	3.81265
O	5.36956	-0.33472	2.66391
H	5.28097	-0.1393	4.69354
H	6.4904	0.90171	3.87937
H	4.68606	1.17368	3.76824
H	6.09419	-0.04009	2.02242
C	-0.6882	2.12688	-4.87349
O	0.31555	2.49017	-5.75296
H	-0.45948	1.14331	-4.44965
H	-0.79728	2.8604	-4.05818
H	-1.63782	2.01947	-5.3664
H	0.93428	3.14001	-5.2509
C	4.8482	3.80762	-2.36403
O	5.26544	2.66494	-3.00285
H	4.9784	3.67453	-1.30397
H	5.4605	4.6881	-2.70042
H	3.80599	3.93963	-2.48446
H	4.7105	2.53502	-3.7697
C	0.56879	4.55236	2.50551
O	0.28228	5.76137	3.30314
H	0.77897	3.79415	3.23925
H	-0.24375	4.28241	1.73822
H	1.45381	4.81796	1.9807
H	0.00617	6.50308	2.65073
C	4.04979	0.35976	-4.34983
O	4.23395	1.41788	-5.26071
H	4.20369	-0.57623	-4.81044
H	4.77924	0.51422	-3.57089
H	3.0931	0.40974	-3.94331
H	3.51186	1.39068	-5.89444
C	-6.16714	4.1159	0.5239
O	-6.10886	2.95696	1.46304
H	-7.14745	4.10872	-0.03653
H	-6.04794	5.07249	1.09299
H	-5.38834	4.05314	-0.25978
H	-6.86795	2.48521	1.42713
C	-3.6412	4.43	3.29781
O	-2.9803	4.73308	4.53953
H	-4.65417	4.75756	3.36448
H	-3.10094	4.98003	2.45703
H	-3.63074	3.32548	3.12808
H	-3.3011	4.02955	5.12263

MP2: -2310.93719
MP2-MBE: -2310.87428
MP2-NN: -2310.87199

Cluster 4:

C	-1.01132	-0.75494	-0.59786
O	0.0	0.0	0.0
H	-1.12986	-1.68393	-0.01903
H	-1.96446	-0.17931	-0.44304
H	-0.73917	-0.98362	-1.6768
H	0.76017	-0.59164	0.09309
C	2.73068	-1.24854	1.6531
O	2.16826	-2.08701	0.60347
H	3.41316	-0.56092	1.19112
H	1.89271	-0.81542	2.1061
H	3.22664	-1.85744	2.37059
H	2.01564	-3.02661	0.8988
C	1.94485	2.69702	0.30405
O	1.25462	2.6539	-0.9255
H	3.00192	2.97468	0.10237
H	1.48496	3.45977	0.87784
H	1.92441	1.76679	0.82872
H	0.41507	2.10541	-0.8318
C	-0.93378	-1.51589	3.44895
O	-1.67281	-0.41829	3.76592
H	0.10051	-1.32296	3.70213
H	-1.20983	-2.42901	3.98115
H	-1.16679	-1.68345	2.39398
H	-1.05753	0.16459	4.21953
C	-2.45952	-4.63905	-2.057
O	-1.71312	-3.39194	-2.20426
H	-1.82291	-5.32594	-2.42563
H	-2.57457	-4.9085	-0.99693
H	-3.4114	-4.6184	-2.65026
H	-2.22283	-2.86593	-2.85433
C	1.47945	-5.15182	2.55224
O	1.59665	-4.57012	1.29104
H	1.38716	-4.40399	3.33755
H	0.54834	-5.80549	2.52657
H	2.33628	-5.79151	2.8147
H	2.02684	-5.24666	0.67319
C	3.77579	0.41748	-2.05017
O	4.08583	-0.66479	-2.91683
H	4.26025	0.24818	-1.07841
H	3.97442	1.44443	-2.4647
H	2.74074	0.40523	-1.84973

H	5.0336	-0.81541	-2.83191
C	0.3668	4.57337	-2.94171
O	-0.99164	4.43343	-2.4965
H	0.9775	5.31192	-2.33772
H	0.87983	3.62557	-3.00061
H	0.38734	5.02753	-3.92863
H	-0.90097	4.24015	-1.52952
C	-5.60139	-2.65012	-3.54666
O	-4.25594	-2.30671	-3.35334
H	-5.90892	-2.52982	-4.61199
H	-5.77629	-3.67756	-3.23233
H	-6.13842	-2.00753	-2.9376
H	-4.28121	-1.34093	-3.48959
C	1.51763	-1.67885	-4.35834
O	2.63635	-1.30909	-5.15921
H	0.74556	-2.07358	-4.99729
H	1.75182	-2.47823	-3.6999
H	1.08158	-0.85946	-3.81186
H	3.36318	-1.48406	-4.56596
C	-4.73166	-0.38947	2.06556
O	-5.41155	0.84679	2.32296
H	-3.74158	-0.19621	1.71558
H	-4.66654	-0.96633	2.98717
H	-5.31285	-0.91203	1.26865
H	-5.92824	1.05919	1.58831
C	1.17429	1.51456	-6.16087
O	-0.06278	2.09245	-5.8525
H	1.61552	1.00279	-5.33866
H	1.04376	0.78859	-6.96143
H	1.88392	2.36799	-6.49128
H	-0.67574	1.47795	-6.21649
C	5.24598	0.78171	3.07486
O	5.96769	0.09143	1.96153
H	4.20566	1.09789	2.6642
H	5.13743	0.0866	3.93076
H	5.77642	1.73328	3.2728
H	5.96405	-0.83476	2.20329
C	5.92259	-2.93186	-0.86718
O	5.05775	-3.83355	-0.37649
H	5.39471	-2.19684	-1.39548
H	6.55047	-2.52322	-0.03051
H	6.5793	-3.47406	-1.47743
H	4.26904	-3.27212	-0.07473
C	-0.18233	3.76042	4.03339
O	-0.68219	5.02131	3.97284
H	0.22087	3.60321	4.9895
H	-0.97465	3.09516	3.79824
H	0.65316	3.66517	3.23979
H	-1.31901	5.12677	3.31801

C	-3.60266	1.42723	-4.33703
O	-4.51476	0.40393	-4.58404
H	-2.71641	0.98783	-3.81347
H	-3.25305	1.83463	-5.3414
H	-4.14323	2.15092	-3.72013
H	-4.88202	0.55227	-5.45216
C	4.54749	4.64374	-1.93295
O	4.57097	4.76206	-0.55078
H	5.30743	5.33072	-2.34401
H	4.719	3.62971	-2.1239
H	3.62473	5.03538	-2.34928
H	5.23731	4.06837	-0.26253
C	7.09442	2.00857	-1.13126
O	6.16055	2.52336	-0.18794
H	6.94209	0.94563	-1.19548
H	6.89128	2.37053	-2.13423
H	8.15728	2.20954	-0.88133
H	5.90696	1.77174	0.37098
C	1.09681	-6.86715	-1.2274
O	2.36282	-6.34494	-0.90143
H	0.53722	-6.26004	-1.95636
H	1.24986	-7.76701	-1.7841
H	0.50873	-7.15523	-0.36079
H	2.35229	-5.40181	-1.21465
C	6.85797	-2.87329	3.43292
O	5.61598	-2.80317	2.718
H	6.71501	-2.91277	4.47625
H	7.26384	-3.82062	3.0815
H	7.46962	-2.08107	3.17729
H	5.41765	-3.6923	2.46517

MP2: -2310.95301
 MP2-MBE: -2310.89366
 MP2-NN: -2310.89384

Cluster 5:

C	0.44737	1.33852	-0.23527
O	0.0	0.0	0.0
H	-0.20264	2.00045	0.36996
H	1.50908	1.41937	0.01395
H	0.27262	1.57616	-1.2803
H	-0.60718	0.01492	0.74568
C	-0.41706	0.23215	4.02639
O	-0.27498	0.11294	2.59164
H	-0.73723	1.23448	4.35753
H	-1.14283	-0.47769	4.28447

H	0.5569	0.03175	4.58236
H	0.13293	-0.74566	2.5012
C	2.13439	-2.1615	-2.91751
O	2.56904	-0.904	-2.49943
H	1.44168	-2.59915	-2.19568
H	1.63258	-2.07538	-3.88719
H	2.96331	-2.81639	-3.06326
H	1.80807	-0.49219	-2.10423
C	-3.60449	-1.0935	-0.27931
O	-3.93805	0.14421	0.34567
H	-3.22417	-0.91568	-1.30232
H	-2.90621	-1.59734	0.24357
H	-4.48042	-1.6633	-0.33782
H	-4.67636	0.03321	0.93599
C	-3.76386	2.46926	-2.679
O	-2.30899	2.53258	-2.53163
H	-4.27898	2.69962	-1.69242
H	-4.12117	3.19027	-3.4323
H	-3.99319	1.43911	-2.98058
H	-2.01867	1.88285	-1.86134
C	-1.99586	-4.41073	-2.68267
O	-1.13229	-3.35163	-2.40871
H	-1.44739	-5.21591	-3.11516
H	-2.37952	-4.72141	-1.69168
H	-2.9137	-4.13973	-3.32867
H	-0.35199	-3.63187	-1.91196
C	-2.9509	2.56776	1.92526
O	-1.92735	3.4321	2.27054
H	-3.9187	2.9591	2.13936
H	-2.8538	2.52401	0.86363
H	-2.82591	1.61709	2.3935
H	-2.09394	3.85264	3.15912
C	3.31244	-1.26664	0.75227
O	4.68906	-1.63161	0.69636
H	2.71933	-2.1399	0.82408
H	3.15726	-0.69662	1.63824
H	2.99856	-0.70059	-0.11334
H	5.02685	-1.26547	-0.14009
C	3.43389	-3.08772	4.0839
O	2.3193	-2.18366	3.93122
H	3.24895	-3.98313	4.73142
H	3.7214	-3.42541	3.07532
H	4.32789	-2.61328	4.44652
H	2.4168	-1.51179	4.65169
C	1.91787	3.06037	2.68895
O	0.85476	4.00063	3.00162
H	2.38558	3.21944	1.72046
H	2.66048	2.98486	3.4638
H	1.49723	2.15175	2.70591

H	-0.01822	3.62281	2.82994
C	1.14775	1.76053	-5.2788
O	-0.21723	2.0627	-4.68946
H	1.03597	1.54475	-6.35299
H	1.83962	2.61232	-5.05191
H	1.50792	0.86017	-4.79752
H	0.01494	2.63535	-3.95702
C	0.40365	4.91696	-1.57381
O	1.28446	5.07157	-0.4451
H	-0.17269	5.81398	-1.67873
H	0.98966	4.70664	-2.44576
H	-0.27704	4.03049	-1.41142
H	1.77359	5.89627	-0.5664
C	0.70976	-6.20046	-0.52003
O	1.64083	-5.10944	-0.30076
H	0.03387	-6.13767	-1.38112
H	1.23411	-7.13762	-0.6665
H	0.1266	-6.30886	0.41902
H	2.51599	-5.50549	-0.43928
C	-0.34081	-4.09264	5.28331
O	-0.06994	-2.7829	4.99196
H	-0.87331	-4.54272	4.33226
H	0.55789	-4.64973	5.54497
H	-1.12669	-4.1607	6.09837
H	0.68158	-2.77825	4.408
C	-1.50548	-1.12704	-4.48198
O	-1.76216	-0.18036	-5.49255
H	-0.66831	-0.86556	-3.8079
H	-2.45009	-1.15718	-3.87401
H	-1.24385	-2.08779	-4.96932
H	-1.0962	0.46274	-5.30625
C	6.96184	-0.62599	-2.09589
O	5.58719	-1.16338	-2.03966
H	7.65452	-1.23492	-1.55566
H	7.34352	-0.62573	-3.13499
H	6.92089	0.46606	-1.8247
H	5.58519	-1.92103	-2.58931
C	4.53689	2.67609	-0.0651
O	5.38456	2.62309	0.99964
H	4.87366	1.93771	-0.7992
H	3.53875	2.43862	0.28703
H	4.56226	3.65034	-0.46915
H	6.22895	2.50273	0.61156
C	-6.65382	0.18213	-2.15226
O	-5.69993	-0.51947	-2.90854
H	-7.61917	-0.28385	-2.33404
H	-6.43444	0.01596	-1.11656
H	-6.67538	1.23431	-2.44109
H	-6.16856	-0.82798	-3.67227

C	-2.95469	0.33162	6.34466
O	-3.52147	1.05646	5.32414
H	-3.74357	-0.09401	6.97537
H	-2.39408	-0.44934	5.92689
H	-2.23926	1.03396	6.84445
H	-4.36356	1.30123	5.67745
C	-2.81761	-3.7154	2.99362
O	-3.54411	-3.75011	4.20977
H	-1.78731	-3.33676	3.20966
H	-2.79183	-4.70027	2.74911
H	-3.37899	-3.1396	2.21055
H	-3.2885	-4.52554	4.58791

MP2: -2310.92133
 MP2-MBE: -2310.86089
 MP2-NN: -2310.85704

Data for Table 2:

Coordinations of the chair, bowl and chain methanol trimer:

chair:

C	-1.6993777421	-1.9493245121	0.2451510954
O	-0.6068322618	-1.3655031864	-0.4399570952
H	-1.4113842738	-2.9560679795	0.5197737116
H	-1.9521429425	-1.4037460454	1.1518852206
H	-2.5819761194	-2.0061586243	-0.3869348923
H	-0.8408400079	-0.4451009767	-0.6593129256
C	-1.3033875524	2.1389523152	0.2988080259
O	-0.5654204979	1.3684866689	-0.6328922793
H	-2.2873581029	2.3049143074	-0.1215598716
H	-1.4143274914	1.6279016959	1.2529853616
H	-0.8386318813	3.1056050547	0.4747205965
H	0.2921491240	1.1546012832	-0.2209761717
C	2.7217014968	-0.2293042530	-0.1151182004
O	1.5075228193	0.0462391390	0.5626608918
H	3.3840391807	0.6109036636	0.0499374839
H	3.1994742129	-1.1246590088	0.2739134897
H	2.5701122051	-0.3490141249	-1.1850780376
H	0.8851084068	-0.6749015179	0.3591083715

bowl:

C	-2.3710459720	0.1090758151	0.4961585526
O	-1.5862223790	-0.0519982293	-0.6702587451
H	-3.0426551607	-0.7379326084	0.5570774645
H	-1.7639211679	0.1324238010	1.3996312734
H	-2.9680465877	1.0166168845	0.4550197669
H	-0.9464976774	0.6819568637	-0.7039635768
C	1.2691074015	1.9655615803	0.4969479632
O	0.7533134369	1.3899569915	-0.6886264525
H	0.8722258570	2.9701351233	0.5713674092
H	0.9714423255	1.4111607262	1.3855225032
H	2.3541588983	2.0273021319	0.4732591945
H	1.0664716627	0.4683554001	-0.7315144202
C	1.0979460445	-2.0678122210	0.5035988945
O	0.8320597666	-1.3592672487	-0.6924308133
H	2.1693271973	-2.2103492474	0.5672518107
H	0.7702956414	-1.5205141656	1.3859784608
H	0.6220494388	-3.0451746144	0.5044746955
H	-0.1237784658	-1.1736124058	-0.7192125804

chain:

C	2.7275862725	0.7668859375	-0.1356699229
O	1.3349746453	0.9549661010	-0.0296681713
H	3.1488954479	1.6626859344	-0.5765240271
H	3.1985294915	0.6144582077	0.8342836195
H	2.9839955365	-0.0759331683	-0.7770636539
H	0.9544939742	0.1466365353	0.3550947903
C	0.1404178218	-2.1186985851	-0.4348658653
O	-0.0253994948	-1.3188503998	0.7242740606
H	1.0556919410	-2.6842796233	-0.3110826409
H	-0.6812997195	-2.8189067618	-0.5591529858
H	0.2250108941	-1.5115333514	-1.3337227493
H	-0.8826107866	-0.8695005660	0.6309290688
C	-1.9090676129	1.4962797033	-0.1986377198
O	-2.2611431108	0.1491375843	0.1214761188
H	-0.8716701178	1.4830948826	-0.5031544312
H	-2.5227009471	1.8753302504	-1.0102988453
H	-2.0070723562	2.1467012596	0.6650675747
H	-3.1463645615	0.1436984984	0.4884050058

Data for Figure 5:

Coordinations (angstrom) and energies (a.u.) of the original dimer/cluster and methanol dimer/cluster with one methanol rotated:

Original Dimer:

C	-1.01132	-0.75494	-0.59786
O	0.0	0.0	0.0
H	-1.12986	-1.68393	-0.01903
H	-1.96446	-0.17931	-0.44304
H	-0.73917	-0.98362	-1.6768
H	0.76017	-0.59164	0.09309
C	2.73068	-1.24854	1.6531
O	2.16826	-2.08701	0.60347
H	3.41316	-0.56092	1.19112
H	1.89271	-0.81542	2.1061
H	3.22664	-1.85744	2.37059
H	2.01564	-3.02661	0.8988

MP2-MBE 2-body: -0.00747

NN-MBE 2-body: -0.00760

Dimer with one methanol rotated:

C	-1.01132	-0.75494	-0.59786
O	0.0	0.0	0.0
H	-1.38559922	-0.19383449	-1.46802894
H	-0.51122189	-1.66876112	-1.02050386
H	-1.84610135	-0.94625853	0.14847036
H	-0.36834806	0.88413106	0.13854258
C	2.73068	-1.24854	1.6531
O	2.16826	-2.08701	0.60347
H	3.41316	-0.56092	1.19112
H	1.89271	-0.81542	2.1061
H	3.22664	-1.85744	2.37059
H	2.01564	-3.02661	0.8988

MP2-MBE 2-body: 0.00139

NN-MBE 2-body: 0.00166

Original Cluster:

C	-1.01132	-0.75494	-0.59786
O	0.0	0.0	0.0
H	-1.12986	-1.68393	-0.01903
H	-1.96446	-0.17931	-0.44304
H	-0.73917	-0.98362	-1.6768
H	0.76017	-0.59164	0.09309
C	2.73068	-1.24854	1.6531
O	2.16826	-2.08701	0.60347
H	3.41316	-0.56092	1.19112
H	1.89271	-0.81542	2.1061
H	3.22664	-1.85744	2.37059
H	2.01564	-3.02661	0.8988
C	1.94485	2.69702	0.30405
O	1.25462	2.6539	-0.9255
H	3.00192	2.97468	0.10237
H	1.48496	3.45977	0.87784
H	1.92441	1.76679	0.82872
H	0.41507	2.10541	-0.8318
C	-0.93378	-1.51589	3.44895
O	-1.67281	-0.41829	3.76592
H	0.10051	-1.32296	3.70213
H	-1.20983	-2.42901	3.98115
H	-1.16679	-1.68345	2.39398
H	-1.05753	0.16459	4.21953
C	-2.45952	-4.63905	-2.057
O	-1.71312	-3.39194	-2.20426
H	-1.82291	-5.32594	-2.42563
H	-2.57457	-4.9085	-0.99693
H	-3.4114	-4.6184	-2.65026
H	-2.22283	-2.86593	-2.85433
C	1.47945	-5.15182	2.55224
O	1.59665	-4.57012	1.29104
H	1.38716	-4.40399	3.33755
H	0.54834	-5.80549	2.52657
H	2.33628	-5.79151	2.8147
H	2.02684	-5.24666	0.67319
C	3.77579	0.41748	-2.05017
O	4.08583	-0.66479	-2.91683
H	4.26025	0.24818	-1.07841
H	3.97442	1.44443	-2.4647
H	2.74074	0.40523	-1.84973
H	5.0336	-0.81541	-2.83191
C	0.3668	4.57337	-2.94171
O	-0.99164	4.43343	-2.4965
H	0.9775	5.31192	-2.33772
H	0.87983	3.62557	-3.00061
H	0.38734	5.02753	-3.92863

H	-0.90097	4.24015	-1.52952
C	-5.60139	-2.65012	-3.54666
O	-4.25594	-2.30671	-3.35334
H	-5.90892	-2.52982	-4.61199
H	-5.77629	-3.67756	-3.23233
H	-6.13842	-2.00753	-2.9376
H	-4.28121	-1.34093	-3.48959
C	1.51763	-1.67885	-4.35834
O	2.63635	-1.30909	-5.15921
H	0.74556	-2.07358	-4.99729
H	1.75182	-2.47823	-3.6999
H	1.08158	-0.85946	-3.81186
H	3.36318	-1.48406	-4.56596
C	-4.73166	-0.38947	2.06556
O	-5.41155	0.84679	2.32296
H	-3.74158	-0.19621	1.71558
H	-4.66654	-0.96633	2.98717
H	-5.31285	-0.91203	1.26865
H	-5.92824	1.05919	1.58831
C	1.17429	1.51456	-6.16087
O	-0.06278	2.09245	-5.8525
H	1.61552	1.00279	-5.33866
H	1.04376	0.78859	-6.96143
H	1.88392	2.36799	-6.49128
H	-0.67574	1.47795	-6.21649
C	5.24598	0.78171	3.07486
O	5.96769	0.09143	1.96153
H	4.20566	1.09789	2.6642
H	5.13743	0.0866	3.93076
H	5.77642	1.73328	3.2728
H	5.96405	-0.83476	2.20329
C	5.92259	-2.93186	-0.86718
O	5.05775	-3.83355	-0.37649
H	5.39471	-2.19684	-1.39548
H	6.55047	-2.52322	-0.03051
H	6.5793	-3.47406	-1.47743
H	4.26904	-3.27212	-0.07473
C	-0.18233	3.76042	4.03339
O	-0.68219	5.02131	3.97284
H	0.22087	3.60321	4.9895
H	-0.97465	3.09516	3.79824
H	0.65316	3.66517	3.23979
H	-1.31901	5.12677	3.31801
C	-3.60266	1.42723	-4.33703
O	-4.51476	0.40393	-4.58404
H	-2.71641	0.98783	-3.81347
H	-3.25305	1.83463	-5.3414
H	-4.14323	2.15092	-3.72013
H	-4.88202	0.55227	-5.45216

C	4.54749	4.64374	-1.93295
O	4.57097	4.76206	-0.55078
H	5.30743	5.33072	-2.34401
H	4.719	3.62971	-2.1239
H	3.62473	5.03538	-2.34928
H	5.23731	4.06837	-0.26253
C	7.09442	2.00857	-1.13126
O	6.16055	2.52336	-0.18794
H	6.94209	0.94563	-1.19548
H	6.89128	2.37053	-2.13423
H	8.15728	2.20954	-0.88133
H	5.90696	1.77174	0.37098
C	1.09681	-6.86715	-1.2274
O	2.36282	-6.34494	-0.90143
H	0.53722	-6.26004	-1.95636
H	1.24986	-7.76701	-1.7841
H	0.50873	-7.15523	-0.36079
H	2.35229	-5.40181	-1.21465
C	6.85797	-2.87329	3.43292
O	5.61598	-2.80317	2.718
H	6.71501	-2.91277	4.47625
H	7.26384	-3.82062	3.0815
H	7.46962	-2.08107	3.17729
H	5.41765	-3.6923	2.46517
C	-4.97723	-3.41828	0.01543
O	-5.64784	-3.75869	1.19179
H	-4.29541	-4.22027	-0.26302
H	-5.67829	-3.23366	-0.78703
H	-4.43842	-2.4768	0.25214
H	-6.09191	-2.98349	1.58662
C	2.82249	-3.49932	5.40684
O	1.61206	-3.17302	5.90951
H	3.54436	-2.92047	5.96701
H	2.95257	-4.61299	5.52222
H	2.90335	-3.23942	4.36196
H	1.77898	-3.02182	6.85248
C	1.62469	6.99204	2.22698
O	2.66875	6.23468	1.64463
H	1.59627	6.69949	3.24604
H	1.91128	8.0211	2.19319
H	0.6353	6.8086	1.76039
H	2.73569	6.5616	0.74904
C	-2.28908	6.36695	1.75058
O	-3.0902	5.69177	2.71912
H	-2.96104	6.77122	0.96571
H	-1.67709	7.10213	2.24818
H	-1.58975	5.63449	1.28376
H	-3.84455	6.33797	2.88716
C	-2.53391	4.75811	-5.06979

O	-3.45579	4.64838	-4.00375
H	-1.57457	4.9226	-4.68851
H	-2.52608	3.85343	-5.64143
H	-2.82029	5.64276	-5.72071
H	-3.01391	4.27895	-3.26962
C	2.16401	-5.90995	-4.70303
O	0.83291	-5.66097	-4.30028
H	2.39051	-5.08509	-5.44496
H	2.85911	-5.86661	-3.89105
H	2.30632	-6.89401	-5.15754
H	0.43496	-5.17899	-5.01717
C	-3.81665	3.09981	4.54003
O	-4.36298	2.764	5.79736
H	-2.87223	2.6136	4.28815
H	-4.58225	3.10808	3.82938
H	-3.47132	4.09671	4.66394
H	-3.66699	2.43674	6.38038
C	-5.29729	5.81231	-0.75991
O	-6.00296	5.21647	-1.81236
H	-5.97377	6.36693	-0.09183
H	-4.86141	5.01889	-0.16108
H	-4.50927	6.35223	-1.12302
H	-6.71932	5.8217	-2.04364
C	5.22368	0.3023	-5.95085
O	4.9352	-0.91755	-6.4902
H	6.25459	0.44597	-6.08902
H	4.66578	0.97858	-6.50617
H	4.99031	0.38337	-4.89499
H	4.043	-1.19642	-6.24553
C	1.02064	1.26925	6.86251
O	1.40241	2.18256	7.81202
H	0.93271	1.78489	5.91117
H	1.80696	0.54452	6.72532
H	0.08271	0.84072	7.21037
H	1.75931	1.68301	8.56688
C	-2.40571	-0.59349	6.8744
O	-1.74189	-1.03037	8.01134
H	-1.61951	-0.42193	6.1354
H	-3.06928	-1.36406	6.43174
H	-2.97964	0.29187	7.04597
H	-2.09456	-0.60512	8.82191
C	-6.59096	1.98603	-2.04965
O	-7.29283	3.01982	-2.61207
H	-6.22276	1.30574	-2.74397
H	-5.76895	2.33738	-1.49943
H	-7.32701	1.50117	-1.36332
H	-6.64585	3.76249	-2.67638
C	-1.91508	-0.15128	-8.93453
O	-1.85629	0.87489	-8.05848

H	-1.18736	-0.86983	-8.72394
H	-2.90029	-0.63634	-8.86461
H	-1.70664	0.25327	-9.95145
H	-1.64723	1.72281	-8.58872
C	5.16664	-4.01169	-4.39516
O	6.19616	-4.3488	-3.54618
H	5.02979	-4.7335	-5.16826
H	4.27931	-3.9035	-3.8315
H	5.31289	-3.00643	-4.88214
H	6.27946	-5.26105	-3.61387
C	-4.31099	-3.8336	4.10123
O	-4.73291	-4.4463	5.28534
H	-4.89816	-2.96943	3.81073
H	-3.23787	-3.57056	4.28296
H	-4.3439	-4.64641	3.38879
H	-4.84449	-3.74283	5.89856
C	-7.53916	-2.64226	4.17064
O	-7.53293	-2.49198	2.78329
H	-7.19266	-3.72047	4.33736
H	-6.79415	-2.06112	4.67332
H	-8.57468	-2.45532	4.58007
H	-7.92301	-3.27672	2.41876
C	-1.62396	-5.8615	5.82724
O	-2.44395	-6.46295	4.83886
H	-1.8966	-4.83864	5.90248
H	-1.78759	-6.26861	6.89988
H	-0.52581	-5.92731	5.55614
H	-3.36103	-6.43677	5.16314
C	-2.23908	2.60023	8.874
O	-2.72743	3.09922	7.66879
H	-3.0993	2.42373	9.52554
H	-1.60097	1.74103	8.67754
H	-1.62249	3.38409	9.31582
H	-2.1368	3.78006	7.50581
C	-5.90549	-7.07672	-1.51318
O	-4.79442	-6.95761	-2.33874
H	-5.57734	-7.46994	-0.54992
H	-6.43999	-6.1337	-1.39847
H	-6.52027	-7.79909	-1.98121
H	-4.8306	-7.77104	-2.85741
C	-7.23862	3.2771	4.26082
O	-7.47109	1.88	4.28738
H	-6.6555	3.51006	5.08345
H	-6.5903	3.42037	3.38813
H	-8.15024	3.72987	4.2073
H	-6.85351	1.49377	3.66119
C	-7.87773	-0.24378	-5.34297
O	-7.98612	-0.58915	-3.91508
H	-6.85075	-0.42937	-5.69074

H	-8.51181	-0.86817	-5.89911
H	-8.23322	0.84518	-5.48277
H	-7.32547	-0.05465	-3.42088
C	-6.26227	-2.99085	7.633
O	-5.40767	-2.41274	6.70654
H	-6.35683	-4.07125	7.40591
H	-5.88033	-2.87439	8.63631
H	-7.20708	-2.51148	7.5365
H	-5.42041	-1.46941	6.92285
C	-1.72613	-8.74359	-3.9085
O	-1.7074	-7.46626	-4.62762
H	-2.4778	-9.45456	-4.39882
H	-0.7224	-9.07316	-4.02306
H	-2.03257	-8.64419	-2.88974
H	-0.89069	-7.07249	-4.39688
C	0.78684	-3.38681	9.28877
O	0.8734	-2.1366	8.66042
H	0.81762	-4.1909	8.48471
H	1.67664	-3.62897	9.98015
H	-0.14362	-3.52628	9.87155
H	0.02335	-1.74975	8.47887
C	-5.43613	1.5494	-8.58804
O	-4.76358	1.69411	-7.41473
H	-4.76759	0.99609	-9.25071
H	-6.29384	0.92854	-8.38523
H	-5.68977	2.57684	-9.05461
H	-3.93335	2.21893	-7.57369
C	5.76013	-5.54361	6.05154
O	5.60956	-5.38757	4.57753
H	5.6787	-4.58353	6.61667
H	4.90714	-6.15618	6.39195
H	6.76621	-6.00835	6.18345
H	5.40169	-6.29094	4.25298
C	-2.84651	-7.329	1.47719
O	-2.92488	-8.16154	2.63084
H	-3.26688	-7.86997	0.55523
H	-3.53951	-6.50509	1.59941
H	-1.8447	-6.94618	1.33493
H	-2.82255	-7.53171	3.40755
C	2.3141	6.35404	-7.67805
O	2.69123	5.68614	-6.52281
H	2.91779	7.27229	-7.82454
H	2.46668	5.69094	-8.49099
H	1.28456	6.73246	-7.53125
H	3.59107	5.31175	-6.66127
C	0.48931	5.55081	6.88305
O	-0.61478	6.42218	6.7344
H	1.21525	5.64745	6.06218
H	0.8853	5.82031	7.82507

H	0.15421	4.5717	6.89357
H	-0.68837	6.55795	5.76566
C	5.29657	-6.32525	1.11376
O	5.50972	-7.19656	2.29542
H	4.36473	-6.56198	0.55542
H	5.25825	-5.25933	1.48755
H	6.09478	-6.40702	0.43108
H	6.39457	-7.58468	2.25049
C	-6.11018	4.29319	-5.77628
O	-6.35115	5.17629	-4.64538
H	-6.77418	4.59445	-6.56392
H	-5.08031	4.35868	-6.015
H	-6.31176	3.30619	-5.50494
H	-5.6919	5.04877	-3.9634
C	8.00386	3.99763	4.61057
O	6.90305	3.66157	5.35466
H	8.93917	4.14246	5.21044
H	8.22832	3.25752	3.9022
H	7.71728	4.9482	4.06131
H	6.49932	4.49543	5.52624
C	3.10817	-0.11478	10.42647
O	2.54941	0.05973	9.12999
H	2.30469	-0.00945	11.14852
H	3.45755	-1.13084	10.48832
H	3.85182	0.52683	10.49826
H	1.97292	-0.72199	8.92158
C	-4.98404	7.95441	4.7143
O	-5.37423	7.28183	3.52281
H	-4.69117	9.05827	4.37654
H	-5.76424	7.9639	5.39902
H	-4.12599	7.44858	5.10654
H	-5.12331	7.83045	2.79895
C	-3.75642	-5.13108	-5.8768
O	-3.94379	-6.44174	-6.19232
H	-4.31088	-4.74626	-5.05494
H	-2.71932	-4.9703	-5.60912
H	-3.93637	-4.55407	-6.75809
H	-3.17399	-6.8629	-5.8519
C	4.34842	5.58145	4.51497
O	5.50692	6.24064	5.12166
H	3.49981	6.28363	4.43355
H	4.60388	5.38722	3.45233
H	4.01573	4.73134	4.96932
H	5.22957	7.1376	5.42819
C	1.1657	7.8933	-3.7882
O	0.20492	8.88168	-4.37225
H	0.88299	7.69515	-2.76607
H	1.10843	7.00247	-4.36942
H	2.19201	8.24029	-3.79604

```

H  -0.58485  8.86383  -3.77755
C   0.5485   4.02862  -8.90793
O  -0.57359  3.21664  -9.41396
H   0.1425   4.93928  -8.59201
H   0.95384  3.39196  -8.11725
H   1.28883  4.19438  -9.67482
H  -0.39279  2.96065  -10.29052

MP2-MBE 2-body:  -0.29345   3-body: -0.03386
NN-MBE  2-body:  -0.29304   3-body: -0.03453

```

Cluster with one methanol rotated:

The coordination of other methanol keep the same except the coordination of the first methanol change to:

```

C  -1.01132  -0.75494  -0.59786
O   0.0   0.0   0.0
H  -1.38559922  -0.19383449  -1.46802894
H  -0.51122189  -1.66876112  -1.02050386
H  -1.84610135  -0.94625853   0.14847036
H  -0.36834806   0.88413106   0.13854258

MP2-MBE 2-body:  -0.27364   3-body: -0.03246
NN-MBE  2-body:  -0.27310   3-body: -0.03121

```

Data for Figure 6:

All methanol clusters are sampled from a single large methanol cluster. Methanol molecule in the cluster is ordered by their distance (measure from the oxygen in the molecule) from the original points (0,0,0). Methanol molecule within a certain radius from the original point will be included in the cluster. Therefore, clusters with larger size contains clusters with smaller size.

MP2-MBE total energies and NN-MBE total energies:

Size of Cluster	MP2-MBE	NN-MBE
10	-1155.44154	-1155.44151
20	-2310.89366	-2310.89384
30	-3466.32591	-3466.32547
40	-4621.76219	-4621.76292
50	-5777.23266	-5777.23410
60	-6932.71002	-6932.70915
70	-8088.17355	-8088.17085
80	-9243.59566	-9243.59563
90	-10399.06025	-10399.05967
100	-11554.50101	-11554.50229
110	-12709.98046	-12709.98114
120	-13865.46474	-13865.46515
130	-15020.97045	-15020.97193
140	-16176.44615	-16176.44647
150	-17331.89433	-17331.89380
160	-18487.34892	-18487.34673
170	-19642.80895	-19642.80706
180	-20798.27554	-20798.27417
190	-21953.72671	-21953.72617
200	-23109.16841	-23109.16667

The coordination of the largest size cluster (200 methanol):

C	-1.01132	-0.75494	-0.59786
O	0.0	0.0	0.0
H	-1.12986	-1.68393	-0.01903
H	-1.96446	-0.17931	-0.44304
H	-0.73917	-0.98362	-1.6768
H	0.76017	-0.59164	0.09309
C	2.73068	-1.24854	1.6531
O	2.16826	-2.08701	0.60347
H	3.41316	-0.56092	1.19112
H	1.89271	-0.81542	2.1061
H	3.22664	-1.85744	2.37059
H	2.01564	-3.02661	0.8988
C	1.94485	2.69702	0.30405
O	1.25462	2.6539	-0.9255
H	3.00192	2.97468	0.10237
H	1.48496	3.45977	0.87784
H	1.92441	1.76679	0.82872
H	0.41507	2.10541	-0.8318
C	-0.93378	-1.51589	3.44895
O	-1.67281	-0.41829	3.76592
H	0.10051	-1.32296	3.70213
H	-1.20983	-2.42901	3.98115
H	-1.16679	-1.68345	2.39398
H	-1.05753	0.16459	4.21953
C	-2.45952	-4.63905	-2.057
O	-1.71312	-3.39194	-2.20426
H	-1.82291	-5.32594	-2.42563
H	-2.57457	-4.9085	-0.99693
H	-3.4114	-4.6184	-2.65026
H	-2.22283	-2.86593	-2.85433
C	1.47945	-5.15182	2.55224
O	1.59665	-4.57012	1.29104
H	1.38716	-4.40399	3.33755
H	0.54834	-5.80549	2.52657
H	2.33628	-5.79151	2.8147
H	2.02684	-5.24666	0.67319
C	3.77579	0.41748	-2.05017
O	4.08583	-0.66479	-2.91683
H	4.26025	0.24818	-1.07841
H	3.97442	1.44443	-2.4647
H	2.74074	0.40523	-1.84973
H	5.0336	-0.81541	-2.83191
C	0.3668	4.57337	-2.94171
O	-0.99164	4.43343	-2.4965
H	0.9775	5.31192	-2.33772
H	0.87983	3.62557	-3.00061
H	0.38734	5.02753	-3.92863

H	-0.90097	4.24015	-1.52952
C	-5.60139	-2.65012	-3.54666
O	-4.25594	-2.30671	-3.35334
H	-5.90892	-2.52982	-4.61199
H	-5.77629	-3.67756	-3.23233
H	-6.13842	-2.00753	-2.9376
H	-4.28121	-1.34093	-3.48959
C	1.51763	-1.67885	-4.35834
O	2.63635	-1.30909	-5.15921
H	0.74556	-2.07358	-4.99729
H	1.75182	-2.47823	-3.6999
H	1.08158	-0.85946	-3.81186
H	3.36318	-1.48406	-4.56596
C	-4.73166	-0.38947	2.06556
O	-5.41155	0.84679	2.32296
H	-3.74158	-0.19621	1.71558
H	-4.66654	-0.96633	2.98717
H	-5.31285	-0.91203	1.26865
H	-5.92824	1.05919	1.58831
C	1.17429	1.51456	-6.16087
O	-0.06278	2.09245	-5.8525
H	1.61552	1.00279	-5.33866
H	1.04376	0.78859	-6.96143
H	1.88392	2.36799	-6.49128
H	-0.67574	1.47795	-6.21649
C	5.24598	0.78171	3.07486
O	5.96769	0.09143	1.96153
H	4.20566	1.09789	2.6642
H	5.13743	0.0866	3.93076
H	5.77642	1.73328	3.2728
H	5.96405	-0.83476	2.20329
C	5.92259	-2.93186	-0.86718
O	5.05775	-3.83355	-0.37649
H	5.39471	-2.19684	-1.39548
H	6.55047	-2.52322	-0.03051
H	6.5793	-3.47406	-1.47743
H	4.26904	-3.27212	-0.07473
C	-0.18233	3.76042	4.03339
O	-0.68219	5.02131	3.97284
H	0.22087	3.60321	4.9895
H	-0.97465	3.09516	3.79824
H	0.65316	3.66517	3.23979
H	-1.31901	5.12677	3.31801
C	-3.60266	1.42723	-4.33703
O	-4.51476	0.40393	-4.58404
H	-2.71641	0.98783	-3.81347
H	-3.25305	1.83463	-5.3414
H	-4.14323	2.15092	-3.72013
H	-4.88202	0.55227	-5.45216

C	4.54749	4.64374	-1.93295
O	4.57097	4.76206	-0.55078
H	5.30743	5.33072	-2.34401
H	4.719	3.62971	-2.1239
H	3.62473	5.03538	-2.34928
H	5.23731	4.06837	-0.26253
C	7.09442	2.00857	-1.13126
O	6.16055	2.52336	-0.18794
H	6.94209	0.94563	-1.19548
H	6.89128	2.37053	-2.13423
H	8.15728	2.20954	-0.88133
H	5.90696	1.77174	0.37098
C	1.09681	-6.86715	-1.2274
O	2.36282	-6.34494	-0.90143
H	0.53722	-6.26004	-1.95636
H	1.24986	-7.76701	-1.7841
H	0.50873	-7.15523	-0.36079
H	2.35229	-5.40181	-1.21465
C	6.85797	-2.87329	3.43292
O	5.61598	-2.80317	2.718
H	6.71501	-2.91277	4.47625
H	7.26384	-3.82062	3.0815
H	7.46962	-2.08107	3.17729
H	5.41765	-3.6923	2.46517
C	-4.97723	-3.41828	0.01543
O	-5.64784	-3.75869	1.19179
H	-4.29541	-4.22027	-0.26302
H	-5.67829	-3.23366	-0.78703
H	-4.43842	-2.4768	0.25214
H	-6.09191	-2.98349	1.58662
C	2.82249	-3.49932	5.40684
O	1.61206	-3.17302	5.90951
H	3.54436	-2.92047	5.96701
H	2.95257	-4.61299	5.52222
H	2.90335	-3.23942	4.36196
H	1.77898	-3.02182	6.85248
C	1.62469	6.99204	2.22698
O	2.66875	6.23468	1.64463
H	1.59627	6.69949	3.24604
H	1.91128	8.0211	2.19319
H	0.6353	6.8086	1.76039
H	2.73569	6.5616	0.74904
C	-2.28908	6.36695	1.75058
O	-3.0902	5.69177	2.71912
H	-2.96104	6.77122	0.96571
H	-1.67709	7.10213	2.24818
H	-1.58975	5.63449	1.28376
H	-3.84455	6.33797	2.88716
C	-2.53391	4.75811	-5.06979

O	-3.45579	4.64838	-4.00375
H	-1.57457	4.9226	-4.68851
H	-2.52608	3.85343	-5.64143
H	-2.82029	5.64276	-5.72071
H	-3.01391	4.27895	-3.26962
C	2.16401	-5.90995	-4.70303
O	0.83291	-5.66097	-4.30028
H	2.39051	-5.08509	-5.44496
H	2.85911	-5.86661	-3.89105
H	2.30632	-6.89401	-5.15754
H	0.43496	-5.17899	-5.01717
C	-3.81665	3.09981	4.54003
O	-4.36298	2.764	5.79736
H	-2.87223	2.6136	4.28815
H	-4.58225	3.10808	3.82938
H	-3.47132	4.09671	4.66394
H	-3.66699	2.43674	6.38038
C	-5.29729	5.81231	-0.75991
O	-6.00296	5.21647	-1.81236
H	-5.97377	6.36693	-0.09183
H	-4.86141	5.01889	-0.16108
H	-4.50927	6.35223	-1.12302
H	-6.71932	5.8217	-2.04364
C	5.22368	0.3023	-5.95085
O	4.9352	-0.91755	-6.4902
H	6.25459	0.44597	-6.08902
H	4.66578	0.97858	-6.50617
H	4.99031	0.38337	-4.89499
H	4.043	-1.19642	-6.24553
C	1.02064	1.26925	6.86251
O	1.40241	2.18256	7.81202
H	0.93271	1.78489	5.91117
H	1.80696	0.54452	6.72532
H	0.08271	0.84072	7.21037
H	1.75931	1.68301	8.56688
C	-2.40571	-0.59349	6.8744
O	-1.74189	-1.03037	8.01134
H	-1.61951	-0.42193	6.1354
H	-3.06928	-1.36406	6.43174
H	-2.97964	0.29187	7.04597
H	-2.09456	-0.60512	8.82191
C	-6.59096	1.98603	-2.04965
O	-7.29283	3.01982	-2.61207
H	-6.22276	1.30574	-2.74397
H	-5.76895	2.33738	-1.49943
H	-7.32701	1.50117	-1.36332
H	-6.64585	3.76249	-2.67638
C	-1.91508	-0.15128	-8.93453
O	-1.85629	0.87489	-8.05848

H	-1.18736	-0.86983	-8.72394
H	-2.90029	-0.63634	-8.86461
H	-1.70664	0.25327	-9.95145
H	-1.64723	1.72281	-8.58872
C	5.16664	-4.01169	-4.39516
O	6.19616	-4.3488	-3.54618
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H	4.27931	-3.9035	-3.8315
H	5.31289	-3.00643	-4.88214
H	6.27946	-5.26105	-3.61387
C	-4.31099	-3.8336	4.10123
O	-4.73291	-4.4463	5.28534
H	-4.89816	-2.96943	3.81073
H	-3.23787	-3.57056	4.28296
H	-4.3439	-4.64641	3.38879
H	-4.84449	-3.74283	5.89856
C	-7.53916	-2.64226	4.17064
O	-7.53293	-2.49198	2.78329
H	-7.19266	-3.72047	4.33736
H	-6.79415	-2.06112	4.67332
H	-8.57468	-2.45532	4.58007
H	-7.92301	-3.27672	2.41876
C	-1.62396	-5.8615	5.82724
O	-2.44395	-6.46295	4.83886
H	-1.8966	-4.83864	5.90248
H	-1.78759	-6.26861	6.89988
H	-0.52581	-5.92731	5.55614
H	-3.36103	-6.43677	5.16314
C	-2.23908	2.60023	8.874
O	-2.72743	3.09922	7.66879
H	-3.0993	2.42373	9.52554
H	-1.60097	1.74103	8.67754
H	-1.62249	3.38409	9.31582
H	-2.1368	3.78006	7.50581
C	-5.90549	-7.07672	-1.51318
O	-4.79442	-6.95761	-2.33874
H	-5.57734	-7.46994	-0.54992
H	-6.43999	-6.1337	-1.39847
H	-6.52027	-7.79909	-1.98121
H	-4.8306	-7.77104	-2.85741
C	-7.23862	3.2771	4.26082
O	-7.47109	1.88	4.28738
H	-6.6555	3.51006	5.08345
H	-6.5903	3.42037	3.38813
H	-8.15024	3.72987	4.2073
H	-6.85351	1.49377	3.66119
C	-7.87773	-0.24378	-5.34297
O	-7.98612	-0.58915	-3.91508
H	-6.85075	-0.42937	-5.69074

H	-8.51181	-0.86817	-5.89911
H	-8.23322	0.84518	-5.48277
H	-7.32547	-0.05465	-3.42088
C	-6.26227	-2.99085	7.633
O	-5.40767	-2.41274	6.70654
H	-6.35683	-4.07125	7.40591
H	-5.88033	-2.87439	8.63631
H	-7.20708	-2.51148	7.5365
H	-5.42041	-1.46941	6.92285
C	-1.72613	-8.74359	-3.9085
O	-1.7074	-7.46626	-4.62762
H	-2.4778	-9.45456	-4.39882
H	-0.7224	-9.07316	-4.02306
H	-2.03257	-8.64419	-2.88974
H	-0.89069	-7.07249	-4.39688
C	0.78684	-3.38681	9.28877
O	0.8734	-2.1366	8.66042
H	0.81762	-4.1909	8.48471
H	1.67664	-3.62897	9.98015
H	-0.14362	-3.52628	9.87155
H	0.02335	-1.74975	8.47887
C	-5.43613	1.5494	-8.58804
O	-4.76358	1.69411	-7.41473
H	-4.76759	0.99609	-9.25071
H	-6.29384	0.92854	-8.38523
H	-5.68977	2.57684	-9.05461
H	-3.93335	2.21893	-7.57369
C	5.76013	-5.54361	6.05154
O	5.60956	-5.38757	4.57753
H	5.6787	-4.58353	6.61667
H	4.90714	-6.15618	6.39195
H	6.76621	-6.00835	6.18345
H	5.40169	-6.29094	4.25298
C	-2.84651	-7.329	1.47719
O	-2.92488	-8.16154	2.63084
H	-3.26688	-7.86997	0.55523
H	-3.53951	-6.50509	1.59941
H	-1.8447	-6.94618	1.33493
H	-2.82255	-7.53171	3.40755
C	2.3141	6.35404	-7.67805
O	2.69123	5.68614	-6.52281
H	2.91779	7.27229	-7.82454
H	2.46668	5.69094	-8.49099
H	1.28456	6.73246	-7.53125
H	3.59107	5.31175	-6.66127
C	0.48931	5.55081	6.88305
O	-0.61478	6.42218	6.7344
H	1.21525	5.64745	6.06218
H	0.8853	5.82031	7.82507

H	0.15421	4.5717	6.89357
H	-0.68837	6.55795	5.76566
C	5.29657	-6.32525	1.11376
O	5.50972	-7.19656	2.29542
H	4.36473	-6.56198	0.55542
H	5.25825	-5.25933	1.48755
H	6.09478	-6.40702	0.43108
H	6.39457	-7.58468	2.25049
C	-6.11018	4.29319	-5.77628
O	-6.35115	5.17629	-4.64538
H	-6.77418	4.59445	-6.56392
H	-5.08031	4.35868	-6.015
H	-6.31176	3.30619	-5.50494
H	-5.6919	5.04877	-3.9634
C	8.00386	3.99763	4.61057
O	6.90305	3.66157	5.35466
H	8.93917	4.14246	5.21044
H	8.22832	3.25752	3.9022
H	7.71728	4.9482	4.06131
H	6.49932	4.49543	5.52624
C	3.10817	-0.11478	10.42647
O	2.54941	0.05973	9.12999
H	2.30469	-0.00945	11.14852
H	3.45755	-1.13084	10.48832
H	3.85182	0.52683	10.49826
H	1.97292	-0.72199	8.92158
C	-4.98404	7.95441	4.7143
O	-5.37423	7.28183	3.52281
H	-4.69117	9.05827	4.37654
H	-5.76424	7.9639	5.39902
H	-4.12599	7.44858	5.10654
H	-5.12331	7.83045	2.79895
C	-3.75642	-5.13108	-5.8768
O	-3.94379	-6.44174	-6.19232
H	-4.31088	-4.74626	-5.05494
H	-2.71932	-4.9703	-5.60912
H	-3.93637	-4.55407	-6.75809
H	-3.17399	-6.8629	-5.8519
C	4.34842	5.58145	4.51497
O	5.50692	6.24064	5.12166
H	3.49981	6.28363	4.43355
H	4.60388	5.38722	3.45233
H	4.01573	4.73134	4.96932
H	5.22957	7.1376	5.42819
C	1.1657	7.8933	-3.7882
O	0.20492	8.88168	-4.37225
H	0.88299	7.69515	-2.76607
H	1.10843	7.00247	-4.36942
H	2.19201	8.24029	-3.79604

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C	0.5485	4.02862	-8.90793
O	-0.57359	3.21664	-9.41396
H	0.1425	4.93928	-8.59201
H	0.95384	3.39196	-8.11725
H	1.28883	4.19438	-9.67482
H	-0.39279	2.96065	-10.29052
C	-2.06991	8.23291	-2.15955
O	-2.36238	9.21461	-3.11884
H	-2.57908	8.44419	-1.22168
H	-2.27585	7.24996	-2.62417
H	-0.94774	8.24429	-1.94857
H	-3.13342	8.94369	-3.65651
C	4.4405	3.59578	7.36935
O	3.89657	3.26709	8.65075
H	4.22033	2.80819	6.68572
H	3.93777	4.49825	6.88855
H	5.52147	3.76073	7.39419
H	3.01377	2.85504	8.46222
C	10.12527	3.75535	-4.03544
O	8.85835	3.46284	-3.32671
H	10.83742	4.17961	-3.36902
H	10.61269	2.91037	-4.4044
H	9.97301	4.44874	-4.83109
H	8.83273	3.92017	-2.49546
C	3.07995	-3.05706	-8.66454
O	4.40662	-2.53009	-8.70827
H	2.51977	-2.60711	-9.46335
H	3.12546	-4.07181	-8.89697
H	2.5751	-2.83836	-7.70153
H	4.61788	-2.03997	-7.99381
C	-8.95818	0.38652	1.5048
O	-9.98852	1.25079	1.10816
H	-8.05803	1.04243	1.84597
H	-9.27542	-0.19304	2.3483
H	-8.74918	-0.31758	0.70597
H	-9.91199	1.33301	0.1029
C	-4.63434	7.98989	-5.87111
O	-4.54014	7.90563	-4.44923
H	-5.65249	7.78548	-6.13331
H	-4.38441	8.9805	-6.23856
H	-4.03437	7.28998	-6.31126
H	-4.71076	6.94716	-4.2209
C	-3.10868	5.16267	-9.66734
O	-3.21742	4.17628	-8.67806
H	-2.39031	5.95482	-9.39546
H	-2.74046	4.80778	-10.56812
H	-4.0356	5.68353	-9.82349
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C	5.44956	4.17474	-9.18555
O	4.97852	4.29021	-7.80418
H	5.61316	3.16727	-9.57222
H	4.70725	4.65844	-9.82582
H	6.35402	4.80244	-9.2599
H	5.58279	3.84514	-7.2504
C	2.30674	-6.84385	7.79223
O	2.83619	-5.57085	8.09724
H	2.30903	-7.41013	8.761
H	1.2279	-6.78591	7.34186
H	2.86989	-7.34236	7.07083
H	3.68372	-5.62293	8.46237
C	9.38823	-1.6857	-2.38842
O	9.47347	-1.34352	-3.6981
H	8.48881	-2.24008	-2.12063
H	10.142	-2.39528	-2.22582
H	9.50397	-0.78825	-1.77743
H	8.7415	-0.73138	-3.86925
C	-6.08793	1.38252	8.33993
O	-5.23029	0.33977	8.8302
H	-6.27716	1.17889	7.30934
H	-7.058	1.44375	8.83326
H	-5.54213	2.30346	8.44445
H	-5.07332	0.40557	9.77635
C	-1.62319	10.60378	3.11254
O	-2.42981	9.41669	3.34756
H	-0.68114	10.50521	3.63596
H	-1.41591	10.78595	2.0709
H	-2.15879	11.43504	3.56467
H	-3.32024	9.64387	3.34376
C	-9.44313	-4.17984	-1.38766
O	-8.96523	-4.31982	-2.73153
H	-9.77542	-3.14852	-1.17512
H	-10.2319	-4.88485	-1.13606
H	-8.57437	-4.34724	-0.73405
H	-9.08701	-3.42761	-3.09812
C	10.13211	-4.994	0.86449
O	8.81525	-5.33141	0.70953
H	10.58822	-4.83672	-0.16168
H	10.21446	-4.06873	1.369
H	10.67179	-5.75638	1.45937
H	8.7969	-6.0121	0.02677
C	-10.19778	3.12217	-4.4888
O	-9.51449	2.14282	-3.4848
H	-10.53202	2.49887	-5.37683
H	-11.06318	3.6313	-4.06677
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H	-8.5934	2.49892	-3.39039
C	-1.72564	-4.26984	-9.29138

O	-0.34833	-4.57405	-9.35251
H	-2.28014	-5.20378	-9.34991
H	-1.82997	-3.75462	-8.4017
H	-1.96387	-3.6494	-10.14173
H	-0.23598	-5.47835	-9.1038
C	0.34672	10.72842	-0.72987
O	1.72022	10.23609	-0.93054
H	-0.36184	10.40863	-1.54554
H	-0.00278	10.13881	0.16084
H	0.36114	11.80067	-0.50681
H	2.33589	10.7679	-0.37936
C	0.24063	-11.66905	-1.0071
O	0.9256	-10.45864	-0.82433
H	-0.21897	-12.01356	-0.10505
H	-0.5627	-11.52926	-1.76422
H	0.91266	-12.5429	-1.42379
H	0.84685	-10.17825	0.12251
C	6.92836	6.11985	1.42041
O	8.26547	6.42491	1.55514
H	6.84155	5.0955	1.73369
H	6.2782	6.77217	1.96701
H	6.68082	6.17897	0.29453
H	8.75387	5.56889	1.38108
C	-8.591	5.24827	1.46453
O	-8.39703	5.83016	2.78074
H	-7.75903	4.53689	1.33723
H	-9.51937	4.65319	1.33823
H	-8.51941	6.05163	0.72791
H	-7.99299	6.68425	2.70758
C	6.01312	0.12367	8.04895
O	7.11172	1.02154	7.79947
H	6.14583	-0.52521	8.92303
H	5.17481	0.79037	8.17198
H	5.86194	-0.46446	7.07772
H	6.85649	1.8114	7.34755
C	5.2943	-7.60457	-2.33397
O	6.48531	-7.9319	-3.03622
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H	4.53913	-8.45195	-2.32052
H	5.49505	-7.50363	-1.28741
H	6.32022	-8.42543	-3.90527
C	7.42222	3.34181	-5.79576
O	7.36876	3.00475	-7.14072
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H	6.40991	3.50313	-5.45876
H	7.79011	2.47066	-5.26043
H	8.12606	2.44544	-7.25881
C	4.55115	8.60548	-1.10392
O	4.33175	9.64661	-2.00031

H	5.33376	8.87859	-0.37407
H	3.64384	8.35276	-0.58725
H	4.96172	7.74803	-1.72234
H	3.73911	10.29107	-1.62681
C	-11.29941	-0.48898	-2.28292
O	-10.72016	0.46755	-1.3748
H	-10.83419	-1.4686	-2.19469
H	-12.36005	-0.65703	-2.09858
H	-11.13296	-0.16312	-3.35244
H	-10.57063	1.28451	-1.90554
C	-6.98807	-6.52107	2.51071
O	-8.23012	-6.28601	3.21487
H	-6.6241	-5.52727	2.33501
H	-6.20985	-7.08314	3.1373
H	-7.27467	-7.04899	1.5361
H	-8.01749	-6.39847	4.17241
C	2.9658	-9.35254	1.93407
O	2.0176	-10.46971	2.09733
H	2.4364	-8.49546	1.51246
H	3.30887	-9.13663	2.90881
H	3.7777	-9.6353	1.32107
H	2.54125	-11.25645	2.14383
C	9.60702	-0.56633	1.08888
O	10.92403	-0.10931	0.70688
H	9.57425	-1.64923	0.92064
H	9.41946	-0.45957	2.17105
H	8.8193	-0.06345	0.42298
H	11.53428	-0.91873	0.64869
C	-5.00578	6.06116	7.64463
O	-3.78358	6.6775	7.88458
H	-4.99717	5.46105	6.72845
H	-5.31612	5.52068	8.50587
H	-5.73308	6.84318	7.49974
H	-3.0724	6.15697	7.51906
C	9.55428	-5.20847	3.99131
O	9.51553	-3.84429	4.2073
H	10.39662	-5.37019	3.34961
H	9.74488	-5.73186	4.91427
H	8.60142	-5.52907	3.5843
H	10.42918	-3.46509	4.34987
C	2.71359	0.81919	-9.78182
O	3.35679	1.89217	-10.44094
H	1.73452	1.14319	-9.43102
H	2.50092	0.11672	-10.52639
H	3.38746	0.45151	-9.00753
H	2.86417	2.03579	-11.27458
C	-6.96178	8.86791	-1.58965
O	-7.84572	7.77451	-1.39242
H	-6.76958	8.89977	-2.64748

H	-7.44073	9.73522	-1.21599
H	-6.01108	8.63502	-1.03885
H	-8.35809	7.90433	-0.56365
C	9.35551	2.84066	1.20487
O	10.58063	3.43478	0.80561
H	9.38941	2.82189	2.27714
H	8.52095	3.34567	0.78897
H	9.42848	1.80376	0.90459
H	11.18645	3.67157	1.59004
C	-6.95389	-5.36629	-5.4346
O	-8.35231	-5.48237	-5.0597
H	-6.66028	-4.31457	-5.14408
H	-6.35049	-6.13911	-4.88532
H	-6.79314	-5.47781	-6.51487
H	-8.41914	-5.09247	-4.1562
C	7.09416	7.40131	-3.25629
O	6.35296	8.44313	-3.93779
H	7.84882	7.76364	-2.52443
H	6.46761	6.75541	-2.67628
H	7.5866	6.94605	-4.11469
H	5.51073	8.63868	-3.54076
C	2.19403	-9.79934	-4.65674
O	3.23671	-9.44624	-5.49907
H	2.14227	-9.13438	-3.83023
H	1.25594	-9.77396	-5.29304
H	2.3585	-10.84357	-4.38996
H	3.95415	-9.15093	-4.95589
C	-8.60628	0.00949	6.06611
O	-8.99702	-0.99498	6.96655
H	-8.75151	0.98051	6.5542
H	-7.56901	-0.10836	5.81676
H	-9.1309	-0.19117	5.17434
H	-9.68261	-0.63468	7.56016
C	4.61169	-3.69591	9.62834
O	5.38152	-4.60535	8.96836
H	3.61667	-4.20553	9.81707
H	5.05671	-3.507	10.63895
H	4.50674	-2.74963	8.97132
H	6.33865	-4.37109	9.12648
C	4.29493	-12.05256	-0.78178
O	3.97011	-10.74047	-1.02669
H	4.5494	-12.59281	-1.72791
H	5.13465	-12.12598	-0.13091
H	3.47309	-12.56214	-0.33409
H	2.999	-10.52741	-0.95112
C	9.00513	-0.38868	5.04455
O	10.16167	0.30505	5.38818
H	9.37528	-1.29232	4.41194
H	8.37672	-0.69007	5.96866

H	8.43755	0.19565	4.37521
H	10.91253	-0.26215	5.18725
C	-6.53113	-7.44062	6.08588
O	-7.64973	-6.61731	5.72245
H	-5.55633	-6.98734	5.89411
H	-6.69717	-7.783	7.13375
H	-6.56472	-8.37419	5.44917
H	-7.56339	-5.75943	6.20046
C	-5.43419	-2.21661	-8.54961
O	-6.04281	-2.12616	-9.81106
H	-6.20042	-2.07659	-7.79056
H	-5.0291	-3.19154	-8.44238
H	-4.62344	-1.52344	-8.39236
H	-5.96366	-2.91406	-10.38213
C	-6.59135	-10.35546	0.38226
O	-7.31881	-9.17893	0.58348
H	-6.23089	-10.46986	-0.64702
H	-5.76404	-10.48237	1.11671
H	-7.32774	-11.198	0.49028
H	-7.74756	-9.01513	-0.2992
C	-1.57307	-10.00328	5.00685
O	-2.51113	-10.71487	4.18822
H	-0.52635	-10.33051	4.86649
H	-1.68375	-8.88034	4.80706
H	-1.84282	-10.08385	6.04752
H	-2.95231	-10.0825	3.61548
C	8.83344	-8.58128	3.34275
O	8.20229	-8.31503	2.06775
H	8.16558	-8.16846	4.1733
H	8.96129	-9.66086	3.42818
H	9.8359	-8.10019	3.47292
H	8.83364	-8.48917	1.37497
C	-0.93939	8.0689	-7.61106
O	-2.04056	8.99864	-7.50761
H	-0.15559	8.43954	-6.99546
H	-1.2387	7.07686	-7.28748
H	-0.53718	8.07948	-8.60069
H	-2.09256	9.24667	-6.60066
C	-10.95402	-4.30631	1.9711
O	-11.35212	-2.93257	2.11067
H	-9.9065	-4.43997	1.70904
H	-11.04158	-4.7728	2.88617
H	-11.60664	-4.8321	1.2395
H	-10.54603	-2.43341	2.20434
C	8.41703	-9.44773	-0.75684
O	8.68544	-8.07315	-1.16189
H	8.26892	-10.13429	-1.65541
H	9.27568	-9.95713	-0.19142
H	7.50447	-9.40112	-0.08154

H	8.00521	-7.94195	-1.90954
C	9.41883	-5.76234	-3.02921
O	9.94474	-5.14677	-4.19935
H	8.86682	-5.08783	-2.36643
H	8.70998	-6.5973	-3.24254
H	10.19784	-6.24954	-2.53799
H	10.04433	-4.23365	-4.10944
C	-8.82088	-3.63269	-7.99599
O	-9.46358	-3.10186	-6.80176
H	-8.84448	-4.72847	-7.94571
H	-9.36152	-3.2842	-8.89597
H	-7.80661	-3.23766	-8.07246
H	-10.36579	-3.38636	-6.71464
C	-1.04626	2.32499	-12.57545
O	0.20397	2.07688	-11.93176
H	-1.31715	1.49074	-13.20509
H	-1.83162	2.54832	-11.83713
H	-0.9493	3.22595	-13.22541
H	0.62876	1.33319	-12.43363
C	-3.33923	10.93181	0.19895
O	-3.64689	11.46794	1.45532
H	-2.98214	9.93409	0.42472
H	-4.121	10.92516	-0.55805
H	-2.53857	11.47044	-0.28747
H	-4.2064	12.21019	1.28734
C	-10.60942	3.17166	3.68682
O	-11.4929	2.75548	2.74362
H	-9.74494	3.49029	3.23435
H	-11.07563	4.00659	4.17803
H	-10.42895	2.35767	4.3929
H	-10.98313	2.22651	2.05703
C	-8.63258	3.08409	-8.7272
O	-9.06892	3.33588	-7.37675
H	-7.73837	3.69843	-8.92241
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H	-9.37024	4.25385	-7.2511
C	8.40129	-1.23707	-9.24284
O	7.82957	0.12597	-9.41592
H	7.93335	-1.78285	-8.47226
H	8.17357	-1.78525	-10.12817
H	9.48884	-1.20598	-9.12955
H	6.87019	0.18706	-9.34811
C	-9.82529	-4.3133	8.20067
O	-9.15839	-4.38427	6.95131
H	-9.14967	-4.40858	9.02258
H	-10.29369	-3.3813	8.30291
H	-10.49992	-5.14493	8.26253
H	-9.59039	-3.78745	6.32028

C	12.72544	-2.2243	3.36802
O	11.86637	-1.09263	3.25252
H	12.84802	-2.54144	4.40648
H	12.42019	-2.99287	2.65895
H	13.69683	-1.99261	3.03101
H	12.38485	-0.31081	3.21645
C	-1.93831	4.84528	12.70901
O	-1.54501	4.60387	11.37623
H	-1.21807	5.52815	13.14522
H	-2.94189	5.24851	12.67074
H	-1.90455	3.93078	13.2737
H	-2.24161	4.92236	10.79062
C	-3.88002	-10.49605	-6.99123
O	-4.63352	-9.8155	-5.9359
H	-2.92541	-9.93542	-7.09648
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H	-4.84431	-8.93907	-6.30877
C	4.45035	9.66604	4.8103
O	5.76254	9.5834	5.3085
H	4.14619	8.66326	4.51973
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C	-3.98743	-11.44641	-2.71177
O	-5.08966	-10.79601	-3.28543
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C	-9.20985	7.17208	-4.23655
O	-8.59438	7.10767	-5.48273
H	-9.05771	8.19597	-3.78017
H	-10.31917	7.03128	-4.39846
H	-8.81099	6.39619	-3.62231
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C	-7.89668	-10.35391	-4.79937
O	-7.07898	-9.28229	-4.31493
H	-7.95395	-10.29026	-5.91658
H	-7.44758	-11.22589	-4.42068
H	-8.88648	-10.23876	-4.32193
H	-6.31486	-9.6783	-3.90729
C	1.94458	5.77544	10.95287
O	3.2397	6.06759	10.43522
H	1.66098	6.6385	11.54722
H	1.23346	5.68096	10.107
H	1.98401	4.89208	11.63697
H	3.79332	5.28411	10.62732
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O	-8.58536	-8.93911	-1.73615
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H	-10.39319	-8.06854	-2.02366
H	-7.87635	-8.96296	-2.3587
C	10.74117	0.51239	-7.24901
O	9.72045	1.36071	-7.84631
H	10.28886	-0.33043	-6.69762
H	11.47372	0.11664	-8.01444
H	11.38499	1.09342	-6.50404
H	9.27564	0.82424	-8.54524
C	-5.0602	2.35738	12.7435
O	-4.48333	1.82047	11.60988
H	-5.5599	3.30657	12.43969
H	-5.76291	1.72061	13.16365
H	-4.30217	2.54342	13.52767
H	-3.57627	1.58235	11.87221
C	4.13241	12.92149	0.63581
O	2.93077	12.25994	0.3062
H	4.2907	13.70238	-0.14222
H	3.98738	13.37619	1.6157
H	4.95614	12.27443	0.6733
H	2.56001	12.62803	-0.50449
C	6.55056	-8.67094	-7.168
O	6.107	-9.2902	-5.98778
H	7.62893	-8.85067	-7.28938
H	6.02534	-9.10174	-8.02222
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H	5.61841	-10.05255	-6.18277
C	8.24025	-4.86437	-6.97958
O	9.12806	-5.882	-6.60029
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H	9.37956	-5.71091	-5.66814
C	-9.99477	9.84635	1.43503
O	-9.15996	8.74065	1.13846
H	-9.45305	10.70153	1.19489
H	-10.82449	9.75725	0.75417
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H	-8.54597	8.72068	1.86286
C	2.25947	-10.07566	5.43954
O	2.70076	-10.45842	6.70921
H	1.95421	-10.93716	4.90829
H	1.33202	-9.54118	5.59976
H	3.03265	-9.54214	4.89417
H	3.15689	-9.73177	7.07305
C	1.69798	11.81339	-6.09516
O	0.97584	11.70276	-4.90579

H	2.70881	11.4376	-5.95234
H	1.15819	11.31951	-6.90125
H	1.71176	12.88235	-6.27714
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C	-0.00288	-8.66974	9.46642
O	0.46008	-7.49805	10.29759
H	0.56994	-9.55851	9.84917
H	-1.1013	-8.78696	9.68634
H	0.17626	-8.57183	8.39257
H	1.38961	-7.45857	10.22017
C	-1.03885	0.26681	11.9493
O	-2.0424	1.05163	12.55505
H	-0.65135	0.72492	11.09519
H	-0.21983	0.12121	12.6581
H	-1.43611	-0.69849	11.74045
H	-1.6816	1.42404	13.38202
C	8.66845	-3.50176	10.6331
O	7.54081	-3.22469	9.82862
H	9.56177	-3.62806	9.95024
H	8.97166	-2.68432	11.28083
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H	7.25216	-2.35155	10.05852
C	-5.43386	-0.38889	-12.49568
O	-5.84177	0.5118	-11.44086
H	-6.27593	-0.70865	-12.95193
H	-4.78357	0.10704	-13.26105
H	-4.86634	-1.17305	-12.05293
H	-5.92471	0.01698	-10.65988
C	11.8394	4.85736	4.18123
O	11.99729	3.81501	3.21466
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H	11.15616	5.58667	3.81913
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H	11.9843	2.99284	3.69825
C	10.09806	0.98201	9.32219
O	9.02054	0.02855	9.3783
H	10.66077	1.13212	10.24665
H	10.74964	0.69518	8.48197
H	9.57257	1.96623	9.06697
H	8.39715	0.3317	8.60754
C	1.83043	-4.16362	-11.76773
O	0.66448	-4.9182	-12.06051
H	2.33824	-4.00079	-12.76762
H	1.50615	-3.19365	-11.2508
H	2.55056	-4.63532	-11.05558
H	0.35321	-5.02685	-11.17119
C	-11.74684	-7.87334	2.43833
O	-10.71284	-7.2538	1.80662
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C	8.78437	10.06477	-0.33286
O	7.5243	10.66793	-0.56421
H	9.14227	10.34873	0.67216
H	8.73139	8.97479	-0.35985
H	9.47577	10.41399	-1.14674
H	6.8489	10.27757	0.05224
C	-5.30972	-6.25633	-9.77557
O	-4.88598	-5.49106	-10.804
H	-6.2738	-6.73907	-10.05341
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H	-5.41892	-5.68569	-8.89783
H	-5.60815	-5.37257	-11.41131
C	-2.23582	-6.02411	10.37414
O	-1.54902	-5.93901	11.58882
H	-3.18404	-5.58784	10.42617
H	-1.62365	-5.47871	9.54912
H	-2.35249	-7.07799	10.14832
H	-0.60094	-5.84939	11.47993
C	-11.57778	-6.80183	-4.71643
O	-11.12167	-5.91384	-3.71935
H	-11.29229	-7.81153	-4.46506
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C	9.11852	8.22914	3.88605
O	9.84293	8.26582	2.74559
H	8.16563	8.76351	3.68497
H	9.00373	7.14149	4.16494
H	9.65128	8.66196	4.78356
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C	7.80978	6.66154	-6.96622
O	7.52691	8.04303	-7.17388
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H	8.52347	6.34737	-7.74317
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C	-8.37512	-7.8408	-7.73072
O	-7.00648	-7.84191	-7.95184
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C	4.40972	9.19021	-6.70421
O	3.81851	10.00679	-7.77249
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C	4.69623	-6.27213	-9.9223
O	6.09752	-6.29621	-9.93934
H	4.20793	-6.10097	-8.94401
H	4.34498	-5.57983	-10.68048
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H	6.32632	-5.72201	-10.63348
C	12.33126	0.67259	-2.60152
O	12.63942	0.54713	-4.02023
H	11.64945	-0.14276	-2.33633
H	13.11059	0.56182	-1.97122
H	11.78073	1.61286	-2.45162
H	12.0656	-0.02159	-4.40691
C	13.15671	1.65972	6.07528
O	12.07451	1.998	5.32188
H	13.7262	0.96418	5.47804
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H	11.35383	1.40104	5.52232
C	-6.39683	-5.69196	10.57638
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O	8.91833	-8.98673	-4.32999
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H	9.97033	-10.65927	-5.01838
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H	8.11441	-9.48798	-4.00519
C	5.5913	-11.75679	4.40363
O	6.70471	-10.85587	4.07775
H	4.82526	-11.63371	3.6339
H	5.92541	-12.8207	4.42381
H	5.19779	-11.40532	5.40103
H	6.40793	-10.30313	3.38824
C	-0.97919	-1.56566	-12.43045
O	0.05961	-2.0567	-13.25222
H	-1.82164	-1.12369	-13.03259
H	-1.39679	-2.45917	-11.90664
H	-0.55597	-0.84905	-11.74055
H	0.1232	-2.98728	-13.19919
C	-8.45629	7.13505	6.00276
O	-9.21495	6.7059	7.07055
H	-8.69278	8.13851	5.65526
H	-7.34955	7.15765	6.28488
H	-8.62423	6.45902	5.16224

H	-10.17497	6.70346	6.85493
C	2.11159	5.51632	-12.26119
O	1.0602	6.3447	-11.79667
H	2.75889	5.07915	-11.49074
H	1.5542	4.64786	-12.64193
H	2.68295	5.93503	-13.05234
H	1.40601	7.06785	-11.33453
C	-3.41212	-2.97435	12.14151
O	-2.91901	-1.95545	12.99882
H	-3.13259	-2.74799	11.13207
H	-3.01472	-3.92768	12.40941
H	-4.44809	-2.96731	12.20856
H	-3.70697	-1.46364	13.3433
C	11.01364	6.87112	-2.97747
O	10.91212	6.58778	-4.38804
H	10.36511	7.70971	-2.65852
H	10.76733	6.01037	-2.40779
H	12.03552	7.09681	-2.68819
H	10.80601	7.44807	-4.70484
C	-11.37062	1.74864	8.84858
O	-10.91654	0.82022	7.91583
H	-12.41463	1.56284	9.17253
H	-10.68499	1.75623	9.74958
H	-11.23969	2.72251	8.46196
H	-11.66129	0.75479	7.28306
C	8.51909	5.85955	7.77246
O	9.86676	5.82595	7.20256
H	8.57218	5.39897	8.76808
H	8.22985	6.86189	7.9257
H	7.85127	5.27509	7.12877
H	9.76979	6.06839	6.28792
C	2.51639	-4.55577	13.57568
O	2.64833	-3.34263	12.86616
H	1.61973	-4.72898	14.0297
H	2.66909	-5.34762	12.89843
H	3.2615	-4.61414	14.36912
H	1.7778	-2.88729	12.75108
C	3.41662	-9.99041	10.19175
O	4.10269	-9.02327	9.27813
H	2.49325	-10.24417	9.66875
H	3.98778	-10.85475	10.4718
H	3.18438	-9.42763	11.10106
H	4.63213	-9.55541	8.64286
C	1.26616	-13.40141	2.61321
O	2.37662	-12.96553	3.42664
H	1.66029	-13.52818	1.5799
H	0.8593	-14.3022	3.0785
H	0.4568	-12.65911	2.55907
H	2.00942	-12.58769	4.27636

C	13.81501	1.94352	0.99438
O	13.42985	1.05768	2.05189
H	13.15508	2.72249	0.95546
H	14.8267	2.21604	1.14704
H	13.79928	1.41276	0.12292
H	12.5107	0.7704	1.85142
C	6.12755	-11.26139	7.96053
O	5.67772	-10.07931	7.25739
H	5.43521	-11.56002	8.75922
H	6.18132	-12.12971	7.27908
H	7.16135	-11.02904	8.35611
H	6.4768	-9.77697	6.74225
C	0.13214	-8.39069	-9.06327
O	0.19507	-9.48837	-9.87565
H	0.87038	-8.41735	-8.25895
H	0.36926	-7.52412	-9.72509
H	-0.85117	-8.38163	-8.65052
H	-0.4062	-10.17021	-9.57313
C	11.71478	-3.05174	-5.22499
O	12.00115	-2.29926	-6.32478
H	11.67047	-2.47355	-4.27626
H	10.72674	-3.42648	-5.32421
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H	12.92573	-2.34158	-6.40026
C	-8.2542	3.80932	8.51206
O	-9.31918	4.56505	9.06236
H	-7.76787	3.34595	9.37267
H	-8.60128	3.03163	7.80301
H	-7.53302	4.38377	7.9694
H	-9.61808	5.22662	8.36626
C	-12.40889	2.77643	-0.43663
O	-13.48378	2.49872	-1.3431
H	-12.17964	1.89243	0.18355
H	-11.49182	3.034	-0.94088
H	-12.68859	3.59949	0.18386
H	-13.73424	3.36388	-1.71152
C	-4.45468	12.82646	-3.82681
O	-4.84177	11.95351	-4.85158
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H	-4.20078	13.76215	-4.27804
H	-5.21551	12.89366	-3.06053
H	-4.94151	11.06405	-4.51509
C	-5.17725	10.01745	8.25315
O	-4.56309	9.17709	9.21533
H	-4.5789	10.01266	7.31801
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H	-5.08443	11.04592	8.62243
H	-4.10038	8.53088	8.61711
C	-13.08799	-0.21839	1.52143

O	-13.53004	-1.1961	2.41781
H	-12.87522	-0.76817	0.5973
H	-13.95721	0.4963	1.27203
H	-12.18476	0.29882	1.85325
H	-12.85958	-1.89497	2.38778
C	11.16656	-2.79657	7.30399
O	12.07901	-1.89137	6.63498
H	11.11263	-2.55916	8.3995
H	10.15808	-2.64532	6.82336
H	11.47809	-3.8467	7.0061
H	12.85424	-1.80802	7.19181
C	0.45168	-1.35452	15.21009
O	0.10382	-1.70241	13.8737
H	0.81829	-2.18779	15.85952
H	1.19928	-0.64227	15.17646
H	-0.46176	-0.962	15.68382
H	-0.83718	-2.01729	13.97461
C	-8.04404	6.6874	-8.27078
O	-9.35186	6.16456	-8.39355
H	-8.18376	7.76529	-8.01774
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C	-4.26735	-9.6768	8.32506
O	-4.26499	-9.18406	9.71009
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C	-2.78611	-12.31909	1.03273
O	-3.0278	-13.67028	0.95099
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H	-2.36662	-11.96045	1.96386
H	-2.20647	-12.0001	0.21207
H	-3.4356	-13.98067	1.80884
C	2.34128	13.50968	-3.12116
O	2.51339	13.69213	-1.79845
H	1.27803	13.28059	-3.38504
H	2.6426	14.40312	-3.61816
H	3.01073	12.64228	-3.4443
H	1.7834	14.25775	-1.51412
C	-0.09399	-11.87645	8.05045
O	-1.21416	-11.17502	8.42808
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H	0.04875	-11.77524	6.97578
H	0.84743	-11.66433	8.53969
H	-1.91518	-11.7755	8.78924
C	-0.95593	13.89167	-2.65216
O	-1.54104	13.57494	-3.86111

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H	-1.23178	12.66057	-4.15184
C	-0.85517	8.65279	9.91047
O	-1.92179	9.18454	10.68502
H	-1.07789	8.65543	8.87264
H	0.09913	9.15113	10.10633
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H	-2.75277	9.30615	10.18834
C	8.03162	12.68132	4.20161
O	7.05416	11.73334	3.98126
H	7.57693	13.6035	3.96853
H	8.34621	12.66898	5.25266
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H	6.32036	11.89792	4.62292
C	-1.88966	-13.93282	5.25859
O	-2.25622	-12.78943	5.8899
H	-2.64979	-14.15271	4.51292
H	-0.95619	-13.77623	4.76605
H	-1.88167	-14.71133	5.98887
H	-2.64996	-12.17112	5.25867
C	7.21361	-3.93042	-11.79167
O	7.92154	-4.66466	-10.91627
H	6.34503	-4.59535	-12.09251
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H	8.00218	-4.16258	-10.1311
C	5.85057	-2.42419	13.58706
O	6.37103	-1.45964	12.68796
H	6.52644	-3.33189	13.56787
H	5.74302	-2.02403	14.59878
H	4.83621	-2.64056	13.30655
H	6.81509	-0.84051	13.27185
C	-8.97896	12.19361	-2.55843
O	-7.70952	11.65569	-3.00709
H	-9.51065	11.34332	-2.1721
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H	-7.33877	11.99435	-3.8614
C	-7.87816	11.38398	4.8298
O	-6.60594	11.47897	5.40468
H	-7.85999	11.04299	3.81241
H	-8.55507	10.66558	5.40293
H	-8.25715	12.4209	4.69826
H	-6.69232	12.26847	5.99616
C	-0.64931	11.33081	6.53862
O	-1.40806	12.35471	7.14228
H	-1.04758	10.37424	6.7171

H	-0.59269	11.58344	5.52913
H	0.38106	11.34289	6.90009
H	-1.22903	12.2048	8.10028
C	13.06776	-6.85254	3.24305
O	12.72816	-5.54939	3.62336
H	14.09618	-6.96002	3.46509
H	12.60826	-7.55674	3.87609
H	12.79872	-7.05411	2.22152
H	13.49846	-5.09966	3.87718
C	4.34541	13.70541	4.8296
O	4.65214	12.48472	5.39273
H	4.39848	14.53682	5.52683
H	5.08983	13.84977	4.02297
H	3.26183	13.63855	4.49494
H	4.14513	12.40294	6.19021
C	7.23275	13.35077	-2.35363
O	7.18064	12.09249	-3.05823
H	7.74957	13.28955	-1.32009
H	7.71206	14.12851	-2.96259
H	6.15758	13.66902	-2.16818
H	7.18164	11.43919	-2.29758
C	13.09332	-8.64435	-0.85986
O	11.96432	-7.90647	-1.25564
H	13.00247	-9.60028	-1.44376
H	14.00359	-8.08998	-1.2385
H	13.18133	-8.80246	0.18527
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C	-9.75504	-9.38352	5.49126
O	-10.37485	-8.13538	5.81836
H	-8.77908	-9.51084	5.93677
H	-10.47957	-10.13423	5.79983
H	-9.71787	-9.45304	4.35453
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C	-3.70018	14.90903	-0.21095
O	-4.19456	13.76559	-0.79589
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O	-3.04546	-4.86423	-13.23838
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H	-1.2619	-5.78241	-13.39235
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H	-3.55613	-5.27697	-12.4757
C	8.66357	10.08745	-4.62269
O	9.71719	9.32853	-5.23321
H	8.91215	11.12818	-4.69085
H	7.7069	9.87324	-5.09306

H	8.66896	9.76409	-3.6112
H	10.49544	9.46938	-4.63008
C	6.85954	2.22285	-11.87919
O	6.26395	3.28736	-12.6097
H	6.96232	1.40304	-12.57346
H	7.76902	2.64044	-11.57558
H	6.2444	1.91161	-11.05218
H	6.83768	4.11806	-12.56253
C	12.54303	-4.57143	-2.15292
O	13.69919	-3.82383	-2.62018
H	11.71098	-3.92154	-2.02688
H	12.34088	-5.50237	-2.72321
H	12.78879	-4.98567	-1.20749
H	14.48744	-4.36742	-2.782
C	1.50015	2.55662	13.15129
O	0.77569	2.30817	14.29803
H	0.94651	3.45933	12.67751
H	2.51967	2.79413	13.43167
H	1.43945	1.75903	12.42795
H	0.91002	2.9856	14.95586
C	-2.8376	7.0577	-13.94239
O	-2.85034	6.63031	-12.66081
H	-2.30654	6.39658	-14.53501
H	-3.87979	7.11224	-14.35032
H	-2.36922	8.05169	-13.8711
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