

Supplementary Information

A Framework for Automated Structure Elucidation from Routine NMR Spectra

Zhaorui Huang, Michael S. Chen, Cristian P. Woroch, Thomas E. Markland* and Matthew W. Kanan*

Department of Chemistry, Stanford University, Stanford, California 94305, United States

*Corresponding authors: tmarkland@stanford.edu; mkanan@stanford.edu

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1 Supporting Figures and Tables

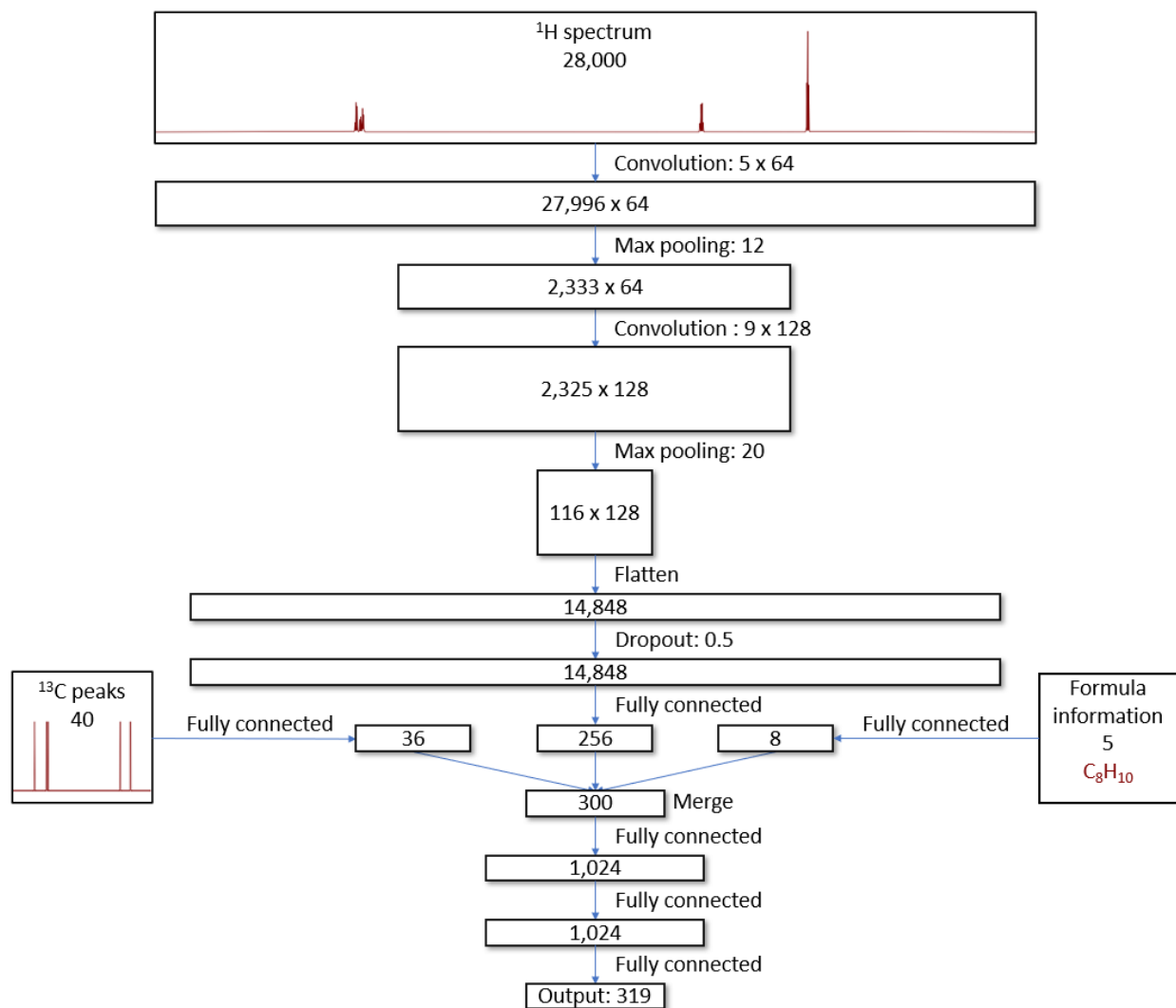


Figure S1. Architecture of the neural network used for substructure prediction.

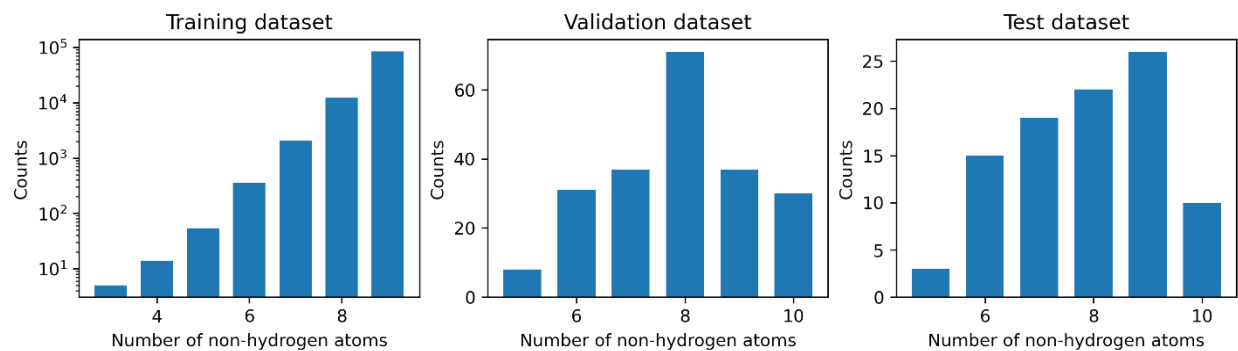


Figure S2. Number of non-hydrogen atoms in the dataset molecules. The distribution of molecules with different numbers of C, N, O atoms for the training, validation, and test datasets. Note that the counts for the training dataset are in log scale for clarity.

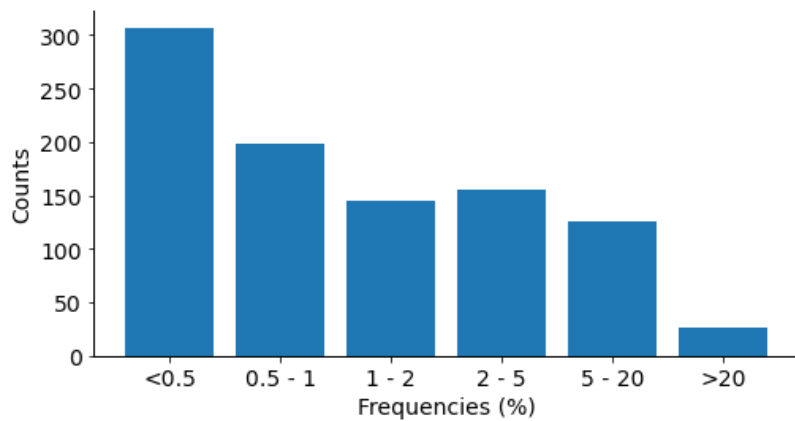


Figure S3. Training set substructure frequencies. The distribution of the frequencies with which the 957 substructures are found in the 100,000 training set molecules.

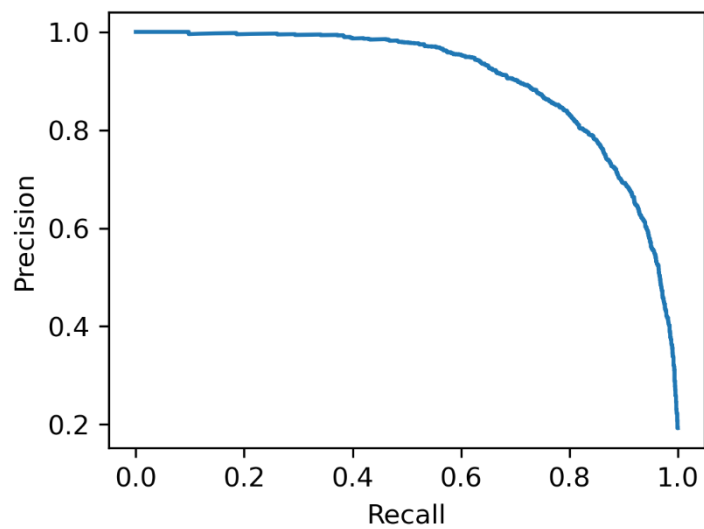


Figure S4. Micro-average precision-recall curve (PRC). The PRC for substructure prediction in the test set. The precision-recall curve area under the curve (PRC-AUC) score is 0.904.

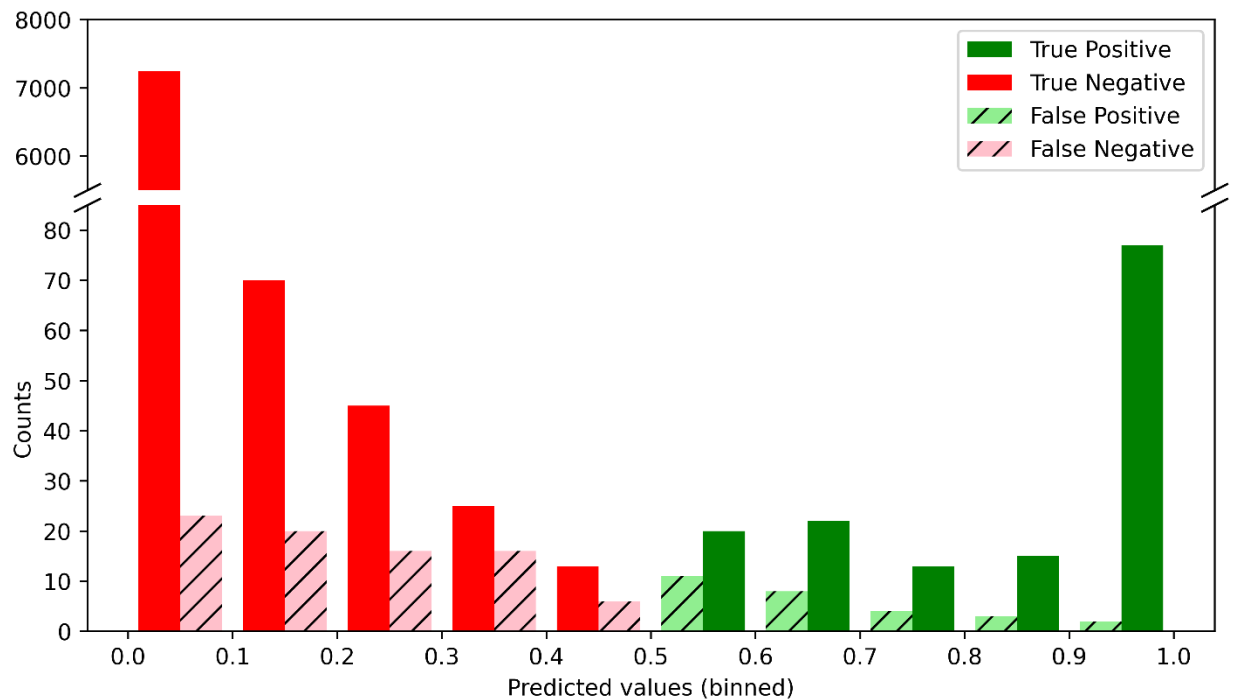


Figure S5. Substructure prediction for larger molecules. Results for substructure prediction for a test set of 8 molecules composed of 1 molecule with 14 non-hydrogen atoms, 5 molecules with 13 non-hydrogen atoms, and 2 molecules with 12 non-hydrogen atoms. The micro-average F_1 score is 0.730 and the PRC-AUC score is 0.829.

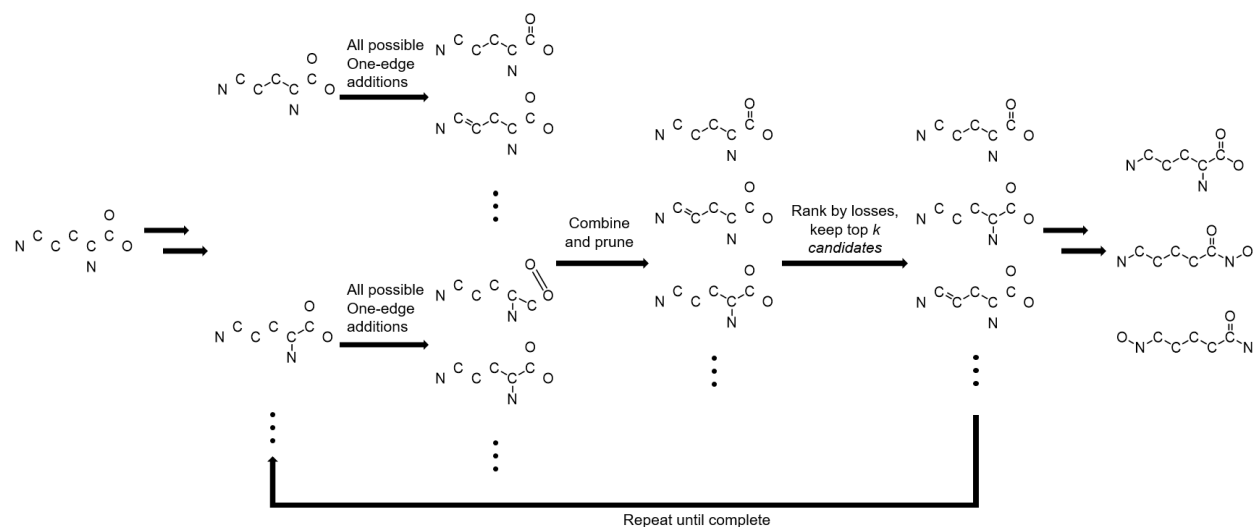


Figure S6. Molecular structure generator schematic. Schematic depiction of the process of generating molecular structures as graphs using a beam search with the substructure probability profile as a guide. At each step, all possible one-edge additions are generated for each partial graph. All the partial graphs are combined, pruned, and their losses are calculated. The losses correspond to the binary cross entropy losses between the actual substructure profile for each partial graph and the substructure probability profile generated by the substructure prediction model. The entire pool is reduced to top k candidates according to the losses and the process is repeated until the graphs are complete according to the molecular formula.

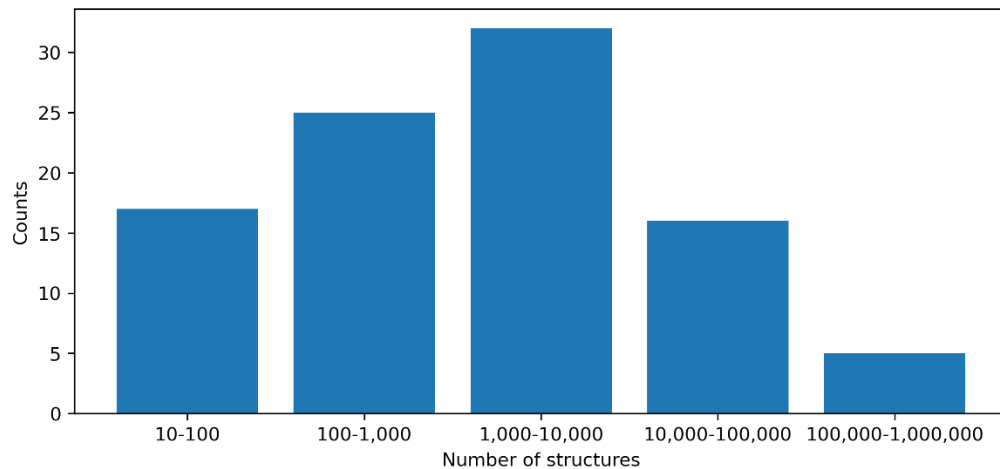


Figure S7. Number of possible constitutional isomers for the test set molecules. The distribution of the number of possible constitutional isomers for the 95 molecules in the test set. The number of possible constitutional isomers for each molecule corresponds to the total number determined by applying the valency rule minus structures that are deemed chemically implausible (See SI Section 3).

Table S1. Structure prediction using different multi-task model configurations. The performance metrics for substructure and molecular structure prediction using different numbers of models to predict the 957 substructures. Note that the results in each row were obtained using a single set of models instead of the ensemble average of 5 models used for the results in Table 1. In addition, for the molecular structure prediction metrics in this table, all possible constitutional isomers were generated for each test set molecule using Open Molecular Generator (OMG) instead of using isomers generated with a beam search using our custom molecular graph generation algorithm.

Dataset	Number of models	Number of tasks per model	Substructure Prediction		Molecular Structure Prediction		
			Micro-Average F ₁ score	PRC-AUC score	Top-1 acc. (%)	Top-10 acc. (%)	Mean reciprocal rank
Validation	1	957	0.828	0.918	82.7	98.1	0.880
	3	319	0.805	0.903	84.6	97.7	0.893
	10	96/93	0.853	0.935	85.5	98.6	0.905
	100	10/7	0.830	0.924	86.4	98.1	0.909
	319	3	0.789	0.893	82.7	97.7	0.883
	957	1	0.777	0.889	81.8	97.7	0.876
Test	1	957	0.761	0.849	62.1	89.5	0.706
	3	319	0.743	0.832	61.1	92.6	0.718
	10	96/93	0.777	0.864	68.4	93.7	0.765
	100	10/7	0.758	0.848	63.2	91.6	0.739
	319	3	0.722	0.806	52.6	91.6	0.671
	957	1	0.704	0.800	55.8	92.6	0.685

Table S2. Results for substructure and molecular structure prediction in the test set with different task-wise early stopping parameters. Training was performed using a single multi-task model that predicts all 957 substructures. The number of task-wise early stopping points was varied using the procedure described in section 3.4. Structure predictions in the test set were performed using the average of 5 predictions from 5 randomly initiated training sessions. For the molecular structure prediction metrics in this table, all possible constitutional isomers were generated for each test set molecular formula using OMG.

Number of stopping points	Total number of models	Substructure Prediction		Molecular Structure Prediction		
		Micro-average F ₁ score	PRC-AUC score	Top-1 accuracy (%)	Top-10 accuracy (%)	Mean reciprocal rank
957	4,785	0.795	0.888	65.3	91.6	0.743
100	500	0.798	0.890	65.3	92.6	0.743
20	100	0.787	0.884	63.2	90.5	0.720
5	25	0.777	0.872	61.1	87.4	0.697
1	5	0.752	0.849	55.8	84.2	0.650

Table S3. List of unstable or unlikely substructures. This list of substructures is used to remove unlikely graphs during graph generation and to remove unlikely structures during the generation of structures using OMG.

SMARTS
[#8H][#8]
[#8H][CX3]([#8)=[#7,#8]
[#8]=[#7][CX4H1]
[#8]=[#7][CX4H2]
[#6X2]=*
[CX3]=[CX3][OH]
[CX4]([#7])([#7])[#7]
[CX4]([#8])([#8])[#8]
[CX4;r3,r4]([#7,#8])[#7,#8]
[#6X2;r3,r4,r5,r6,r7,r8]
[#6X3;r3,r4]
[CX4r3,r4;R2,R3,R4,R5,R6,R7]

Table S4. Test set molecular structure generation using different beam sizes. The effect of beam size (k) on the performance of the molecular generator is indicated by the % of the test cases for which the correct molecular structure is the top-ranking generated structure (Top-1), within the top ten generated structures (Top-10), or not present at all within the k structures (missing). Mean reciprocal rank is defined in section 3.5 below. The last row is result from using the OMG to generate all possible constitutional isomers for each molecular formula.

Beam size	Top-1 (%)	Top-10 (%)	Missing (%)	Mean Reciprocal Rank
1	13.7	13.7	86.3	0.137
5	36.8	37.9	62.1	0.374
25	52.6	58.9	41.1	0.547
100	63.2	74.7	23.2	0.677
500	69.5	91.6	6.3	0.774
1,000	67.4	95.8	2.1	0.777
OMG	68.4	95.8	-	0.777

Table S5. Structure prediction using raw vs processed experimental inputs. Comparison of performance metrics for substructure and molecular structure prediction for the test set when using processed ¹H NMR experimental spectra (peaks for solvent, labile protons, and impurities removed), raw ¹H NMR experimental spectra (no processing), or simulated ¹H spectra as inputs (see SI Section 2.3). For the molecular structure prediction metrics in this table, all possible constitutional isomers were generated for each test set molecular formula using OMG instead of using isomers generated with a beam search using our custom molecular graph generation algorithm.

Experimental Dataset Source	Dataset	Substructure Prediction		Molecular Structure Prediction		
		Micro-Average F ₁ score	PRC-AUC score	Top-1 acc. (%)	Top-10 acc. (%)	Mean reciprocal rank
Processed Experimental	Validation	0.869	0.953	86.9	99.5	0.908
	Test	0.803	0.904	68.4	95.8	0.777
Raw Experimental	Validation	0.785	0.902	72.9	96.3	0.809
	Test	0.728	0.845	56.8	93.7	0.675
Simulated	Validation	0.914	0.979	89.7	100.0	0.936
	Test	0.854	0.941	75.8	96.8	0.838

2 Dataset

2.1 Data processing

The inputs to the substructure prediction model are the ^1H NMR, ^{13}C NMR peaks, and the molecular formula. The ^1H NMR input is a vector of 28,000 numbers representing the intensities from -2 to 12 ppm with 0.0005 ppm resolution. This representation contains information regarding coupling constants and peak shapes, which is typical lost when only using a list of peaks. Since ^1H NMR experimental spectra can have varying resolutions, we map all spectra onto the same set of 28,000 shift values by linearly interpolating between the two closest intensity values to a particular shift value. If the original spectrum does not fully cover the range of shifts from -2 to 12 ppm, the range not covered is assumed to be of zero intensity throughout. Before being input into the model, the ^1H intensities are normalized. First, all negative intensity values are set to zero, thus removing artifacts that are sometimes present, and then the intensities are normalized such that the max intensity has a value of one.

The ^{13}C NMR input to the substructure prediction model is an array of 40 numbers that are either zero or one, representing binned ^{13}C NMR peaks from -2 ppm to 231 ppm. We opted to bin these inputs because typical ^{13}C NMR spectra peaks are decoupled and thus do not have useful information in the peak shapes. Because the intensities of the peaks in routine ^{13}C NMR spectra are not reliable indicators of the relative number of nuclei, we ignore intensity and assign either zero or one for whether there is a peak present in a particular bin of shifts. If for a given molecule multiple peaks are assigned to a single bin, that bin is still set to one for that molecule.

The molecular formula input is an array of 5 numbers. The numbers correspond to the number of each element (H, C, O, and N) and the degree of unsaturation.

Each molecule in our datasets is labeled with a vector where each entry corresponds to one of the 957 substructures and the presence of that substructure in the molecule (0 if that substructure is not in the molecule and 1 if it is). These vectors correspond to the actual substructure profiles for each molecule. The labels are generated using RDkit¹, where full molecular structure graphs are generated using SMILES² and substructure graphs are generated using SMARTS³. The presence of each substructure in a given molecule is determined using RDkit's substructure search function.

The structures of each molecule are represented by canonical SMILES after removing all stereochemistry using RDkit (double bond stereochemistry is also removed).

2.2 Training set

Experimental NMR spectra are usually reported as a list of peaks or as a figure instead of the raw spectral data (intensity vs ppm) needed for an input to our model. We therefore used simulated ^1H and ^{13}C NMR spectra to train the model.

The training set of 99,904 molecules was sampled from a subset of GDB-13⁴ consisting of all GDB-13 molecules with up to 9 C, N, and/or O atoms. More specifically, we randomly sampled 10,526 from the subset of molecules with at least 1 each and fewer than 9 total C and N atoms (the CN subset), 56,842 from the CO subset, and 32,630 from the CNO subset, totaling 99,998. We then removed molecules that are present in the validation or test set from the training set, resulting in 99,904 molecules. The list of the training set structures is available as SMILES in training_smiles.txt. The number of non-hydrogen atoms in the training set molecules ranges from 3 to 9 (**Figure S2**). The molecules in GDB-13 are specified as SMILES strings. OpenBabel⁵ was used to convert the molecules from SMILES to 2D MOL files in order to load the molecules into MestReNova for NMR predictions. The ^1H and ^{13}C NMR spectra for the training set molecules were generated using the MestReNova⁶ NMR prediction function where the solvent was set to CDCl_3 and labile protons were excluded from the ^1H NMR. All other parameters for the prediction of NMR spectra were default parameters.

The simulated training set ^1H NMR spectra were augmented to introduce variability in their peak widths to better reflect the variability in experimental spectra. For each spectrum, a random number, n , was sampled from a normal distribution ($\mu=1$, $\sigma=0.2$). n was rounded to the nearest integer and set to 1 if it is less than 1. Then n spectra were summed together with each spectrum offset by 0.0005 ppm with the center of the peak maintained. This procedure effectively increases the peak widths for some of the spectra.

2.3 Validation and test set

Experimental ^1H NMR data were obtained from the HMDB data base⁷, measurements performed at the Stanford University Department of Chemistry NMR facility, and Scifinder. The spectra collected at Stanford were recorded on a Varian Direct Drive 400 MHz spectrometer, or a Varian Unity Inova 300 MHz spectrometer. Each experimental ^1H spectrum was processed by fitting all of the peaks in the spectrum using the MestReNova software and then removing solvent, impurity, and artifact (i.e. negative) peaks to generate a new spectrum. The new spectrum was then normalized as described above. For predictions using raw spectra in **Table S5**, only a baseline correction was performed before normalizing the data.

Experimental ^{13}C NMR data were obtained from the HMDB data base⁷, SDBS⁸, Sigma-Aldrich, or literature experimental spectra.

The experimental data was randomly split into the validation and test sets while making sure there are no shared molecular structures between the validation and the test set. The validation set consists of 214 total examples with 191 unique molecular structures, so some of the molecular structures have more than one spectrum. The test set consists of 95 unique molecular structures. None of the examples in the test set have more than one stereocenter whereas there are 7 different unique structures with multiple stereocenters in the validation set. The distribution of number of non-hydrogen atoms are shown in **Figure S2**. Molecular structures and NMR spectra of each example in the validation and test set are available in validation_results.pdf and test_results.pdf.

3 Method

3.1 Design of the neural network used for substructure prediction

The overall architecture and inputs are shown in **Figure S1**. The ^1H NMR data is first processed through two sets of a 1-dimensional convolutional layer followed by a pooling layer. This architecture is widely used in image processing⁹. Dropout was applied after flattening the output from the convolutional layer to reduce bias. Then, the output of the dropout layer, the binned ^{13}C peaks, and molecular formula information are each passed through a fully-connected hidden layer and then merged. The merged layer is passed through two more hidden layers to arrive at the outputs. Each node in the output layer uses a sigmoid activation function so that the output is a value between zero and one representing the probability that a given substructure is present.

3.2 Substructure selection

Substructures were selected by two different methods and then they were combined and filtered.

For the first method, two random molecules in the training set were selected and compared. Substructures that could be used to differentiate the two molecules were identified while considering the usefulness of their NMR features. These substructures were used to label the training set. Then, two more molecules that have the same labeling with this set of substructures were then selected at random from the training set and compared. Additional substructures were identified that could differentiate the newly selected molecules. This process was repeated and 727 substructures were obtained this way.

The second method was a more systematic process. A carbon atom was first selected with a given explicit attached hydrogen count, hybridization, and aromaticity. Then, all possible non-hydrogen atoms that the carbon atom can be connected to is iterated. This includes all carbon, oxygen, and nitrogen atoms with different explicit attached hydrogen, hybridization and aromaticity. This process effectively generates all substructures with a non-hydrogen atom bond radius of 1, and about 5,000 substructures were obtained this way.

Finally, duplicate substructures from the two methods were removed by comparing the labels on the 100k training structures. If a substructure had the same labeling for all 100k training structures as another substructure, it was considered to be a duplicate. Substructures with fewer than ~0.2% occurrences rate in were removed. After removing duplicate and rare substructures there were 957 substructures in the final set. The frequencies of the substructures are shown in **Figure S3**.

3.3 Model training and evaluation

The overall substructure prediction model was trained as multiple multi-task models, where each model makes n different substructure predictions. Training set examples were sampled at random without replacement from the 100,000 total examples in the training set until all training set examples had been passed through the models (one epoch) and then the process was repeated until the training was stopped. After each interval of 1,024 training set examples had been passed through the models, the binary cross entropy (BCE) loss was evaluated for the validation set for each of the 957 substructures. This procedure was used because the model can overfit to the training set in the middle of an epoch.

Task-wise early stopping was used to optimize the prediction of each substructure. The training was stopped at a different time for each substructure according to its BCE loss in the validation set. Thus, the training process results in 957 different models with different weights resulting from stopping training at a different time for each substructure. Each model was utilized to predict only a single substructure, even though each model was trained as a multi-task model that generates n substructure predictions. Finally, ensemble learning was used to stabilize the prediction results with respect to erratic predictions from any single model. The models were trained five times as described above using randomly initialized weights and the average value of the five predicted probabilities for each substructure was used. In total, 4,785 models are used to make the 957 substructure predictions using ensemble learning. Since this approach is relatively resource-intensive, we also evaluated performance using fewer models, as described in the next section.

The substructure prediction results were evaluated using the accuracy, micro-average F_1 score, the precision recall curve-area under the curve (PRC-AUC) score. The results for each substructure are shown in detail in **SI Section 4**. The PRC-AUC score was chosen as a metric because it is more suitable for ranking predictions rather than outputting well-calibrated probabilities. For example, consider a set of four molecules that either do (1) or do not (0) contain a particular substructure where the correct assignment is [0, 0, 1, 1] for molecules one through four. If the model's predictions for this substructure for these four molecules was [0.01, 0.02, 0.04, 0.05], then the F_1 score would be 0 (the worst possible F_1 score) if we used a classification threshold of 0.5. However the PRC-AUC would be 1.0 (the best possible PRC-AUC score) since the molecules that actually contain the substructure have higher predicted values than those that do not contain it and hence are ranked correctly. In contrast to area under the receiver operating characteristic curve, PRC-AUC score puts more weight on the positive classes and is a more suitable metric for unbalanced datasets.

3.4 Reducing the number of models used for substructure prediction.

When using task-wise early stopping and ensemble learning (5 initializations) with 957 tasks per model as described above, the result is 4,785 models to predict for the 957 substructures. Since each model is independent, all models can be applied in parallel to speed up predictions if resources allow. However, substructure prediction can be slow if the predictions cannot be performed in parallel. To mitigate this problem, a smaller number of stopping points, n , can be used so that there are only n models to predict

for 957 substructures. For $n = 1$, a single multi-task model that predicts all 957 substructures is stopped at a single time when the BCE loss for all substructure predictions combined in the validation set is minimized. Taking the average result of 5 predictions from 5 random initializations (ensemble learning), only 5 models are used to predict for 957 substructures. However, since different substructures have different optimal stopping times, this method has substantially worse performance compared to having a different stopping point for each substructure (**Table S2**). We therefore evaluated intermediate values of n between 1 and 957 to assess the tradeoffs between speed and prediction performance.

Given a set of x models, each capable of make y predictions, there are x^y different ways of using a subset of those x models to make y predictions. Thus, it is not feasible to assess all possible ways of using a subset of 4,785 models to make 957 predictions. To optimize substructure prediction performance with n stopping points, we developed an iterative process to determine the stopping points. The process starts with a full set 957 models generated by task-wise early stopping of a single multi-task model that predicts for 957 substructures (i.e. stopping training 957 different times). At the start, each model generated by early stopping has an optimal BCE validation set loss value for one substructure as well as 956 BCE loss values for all the other substructures. Next, the increase in validation loss that results from removing each of the models is calculated. This calculation is performed by finding the difference between the BCE validation loss value for the substructure predicted optimally by the model being removed and the BCE loss value for predicting that substructure using the next best model. The model whose removal results in the smallest increase in loss is removed, and the next best model is used to predict for that substructure. Thus, after the first step, 956 models are left, predicting for 957 substructures, where one of the models is used to predict for two substructures. This process is repeated until n models are left. After the first iteration, a model that is removed in subsequent iterations may be a model that is used to predict more than one substructure. In this case, all of the substructures predicted by that model are subsequently predicted by the next best model.

Using this procedure, we evaluated substructure and molecular structure prediction performance as a function of n . The results are presented in **Table S2**. As seen in this table, the performance is similar upon reducing 957 stopping points to 100. A modest reduction in performance is observed upon reducing from 957 stopping points to only 20 stopping points, with the benefit of reducing the computational cost of substructure prediction by a factor of 50.

3.5 Molecular structure generation and evaluation

A ranked list of molecular structures can be generated using the predicted substructure probability profile. To do this, we performed a beam search in molecular structure space using the substructure profile as a heuristic. We frame the problem as a search problem with the molecular structure represented as a graph (**Figure S6**). The nodes of the graph represent the atoms and the edges of the graph represent the bonds in the molecule. Each node has a single property corresponding to the atomic number of the atom it represents and each edge has a property corresponding to the bond order of the bond it represents. Starting with a given number of non-hydrogen atoms, different edges are added one at a time until the graph is complete. First, all possible bonds are considered between any two atoms and of any bond type that is allowed based on the specification of the molecule's degree of unsaturation. This results in several graphs with one added bond. These graphs may include chemically unstable motifs or unlikely motifs. The graphs with such undesired motifs are removed. The set of undesired motifs used can be found in **Table S3**. Each of the remaining graphs are labeled with its corresponding substructure profile and the BCE loss between each graph's substructure profile and the ML-predicted substructure profile is calculated according to the following equation, where N is the total number of substructures, y_i is the label, and \hat{y}_i is the prediction.

$$L = -\frac{1}{N} \sum_{i=0}^N y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)$$

The BCE loss is then used to rank the generated graphs. Using beam search, the top k graphs with the best BCE loss are kept. All possible bonds are added to each of the kept graphs and the process is repeated. When a graph is complete and consistent with the input molecular formula, that graph is added to a list of completed molecular structures that are ranked by the similarity of their substructure profile with

respect to the ML-predicted substructure profile, as quantified by the BCE loss. The accuracy of our structure elucidation framework is evaluated using top-x accuracy metrics, which report the percentage of examples in the validation or test set with the correct structure ranked within the top x candidates. Mean reciprocal rank is also calculated according to the formula below, where r_i is the rank of the correct structure of the i^{th} example ($r_i = 1$ being the best rank).

$$\text{Mean reciprocal rank} = \frac{1}{N} \sum_{i=0}^N \frac{1}{r_i}$$

The results in the main text used a beam size of $k = 1,000$. The effect of varying k is shown in **Table S4**.

As an alternative to our beam search method described above, the Open Molecule Generator (OMG)¹⁰ software can be used to generate all possible constitutional isomers and substructure profiles for a given molecular formula. A ranked list of predicted molecular structures can then be generated by calculating the BCE losses between the substructure profiles for the candidates and our predicted substructure probability profile. It is feasible to use OMG for smaller molecules (<10 non-hydrogen atoms) but it quickly becomes infeasible to generate all possible constitutional isomers for larger molecules because of the number of possibilities increase exponentially with molecular size. We opted to use OMG to generate all candidates for all the molecular formulae in the validation and test sets for the molecular structure prediction results reported in **Tables S1, S2** and **S5** because those tests focused on the accuracy of the ML-predicted substructure probability profiles and not the comprehensiveness of the graph generation algorithm. Structures with undesired motifs were removed and the substructure profiles of the resulting candidate structures were labeled. The BCE losses between the labels of the candidate structures and the predicted substructure profile were used to rank the candidate structures.

3.6 Spectra annotation

To annotate a particular feature in a ^1H or ^{13}C NMR spectrum, a masking method is used. The masking method compares the predicted substructure probability profile of the original input spectra with those of a modified input spectra where the region of interest is masked. The masking is accomplished by replacing the intensities in the region with a line connecting the intensities of the start and the end of the region. The changes in substructure probabilities are ranked and the substructure with greatest decrease in probability is assigned as the predicted substructure for that region.

Spectra annotation results for molecules in the test set are depicted in the accompanying `test_annotation_results.pdf` file. The average substructure probability predictions of 5 set of models with 319 tasks per model was used for the spectra annotation results. An auto peak picking method with an intensity threshold of 0.0025 was used to detect the ^1H NMR regions for each example.

4 Results

4.1 Individual substructure results table

Sorted by number of supports in the test and validation set.

There are 214 examples in validation set and 95 examples in test set.

Acc: accuracy

F1: F₁ score

PRC: PRC-AUC score

Num: number in set

F₁ score and PRC-AUC scores are ill-defined for examples with no positive examples in the set and are left as zero.

SMARTS strings	Validation				Test			
	Acc	F1	PRC	Num	Acc	F1	PRC	Num
[#6H1]	0.888	0.919	0.983	145	0.895	0.923	0.984	64
[OX2H1]	0.935	0.943	0.992	123	0.947	0.959	0.993	61
[CX4H3]	0.972	0.975	0.998	121	0.947	0.950	0.993	52
[#8]=[#6][#8]	0.953	0.949	0.992	99	0.926	0.920	0.995	47
[CX3](=[OX1])O	0.944	0.937	0.993	99	0.916	0.907	0.993	47
[CX3](=[OX1])C	0.953	0.958	0.997	117	0.968	0.968	0.998	46
[CX4H3][#6]	0.995	0.995	1.000	96	0.989	0.988	0.999	43
[CX3](=O)[OX2H1]	0.911	0.885	0.968	86	0.884	0.849	0.973	41
[CX4H2]([#6])[#6]	0.986	0.984	0.999	95	0.937	0.927	0.972	40
[#6H3][#6][#6]	0.986	0.984	1.000	93	0.979	0.974	0.994	39
[#6X3][#6X3]	0.991	0.988	0.999	81	0.989	0.987	1.000	38
[#6X3H1][#6X3H0]	0.977	0.964	0.987	67	0.958	0.941	0.979	34
[#7][#6][#6X3]	0.967	0.951	0.976	71	0.947	0.921	0.993	32
[cH]	0.995	0.991	0.999	59	1.000	1.000	1.000	32
[#8][#6H0][#6H1]	0.836	0.711	0.795	64	0.800	0.667	0.823	31
[#8][#6][#6H2]	0.888	0.829	0.930	68	0.916	0.857	0.947	30
OCC[CH2]	0.921	0.870	0.962	66	0.916	0.857	0.960	30
[#6H1][#6H1]	0.935	0.899	0.966	71	0.916	0.867	0.963	29
[CX4H2][CX4H2]	0.958	0.931	0.989	66	0.926	0.877	0.956	29
[CX4H2]CC=O	0.921	0.857	0.966	58	0.937	0.885	0.970	27
[cH][cH]	0.991	0.982	1.000	57	0.958	0.929	0.994	27
[#6H3][#6H0]	0.977	0.938	0.993	41	0.979	0.963	0.999	27
[cX3H1]([cX3H1])[cX3H0]	0.977	0.954	0.959	54	0.968	0.941	0.994	25
[#6X3][#6X3][#6X3][#6X3]	0.986	0.972	0.997	54	0.947	0.906	0.995	24
[#8]=[#6H0][#6H1]	0.907	0.792	0.921	51	0.884	0.732	0.925	24
[#8][#6][#6][#6X3]	0.916	0.800	0.931	50	0.947	0.898	0.964	24
[#7X3H2]	0.949	0.893	0.964	55	0.905	0.816	0.862	23
[#7][#6][#6][#6X3]	0.977	0.944	0.989	46	0.937	0.864	0.939	23
[#6H3][#6][#6X3]	0.977	0.933	0.991	37	0.905	0.791	0.857	23
[#6H1][#6H2]	0.916	0.842	0.925	58	0.916	0.810	0.919	21
[CX4H2]([CX4H2])[CX4H2]	0.981	0.937	0.986	33	0.968	0.923	0.989	20

[CX4H2][CX3]=O	0.930	0.880	0.965	65	0.905	0.757	0.914	19
O=[CX3][CX4H]	0.953	0.857	0.955	35	0.968	0.914	0.952	19
[#7X3H1]	0.864	0.453	0.604	32	0.779	0.222	0.490	19
[CX4H2]([#6])[O]	0.967	0.904	0.981	36	0.979	0.944	0.988	18
[#7X3][#6H2]	0.986	0.959	0.953	35	0.958	0.882	0.979	17
[#7][#6H2]	0.977	0.932	0.973	35	0.989	0.971	0.985	17
[cX3H1]([cX3H1])[cX3H1]	0.944	0.872	0.949	44	0.947	0.857	0.967	16
[#6X3][#7][#6X3]	0.939	0.800	0.846	34	0.905	0.727	0.860	16
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.902	0.667	0.718	32	0.916	0.692	0.882	16
[#7][#6H0][#6H1]	0.930	0.754	0.841	31	0.958	0.875	0.931	16
[#6X3][#6][#6][#6H3]	0.925	0.800	0.915	42	0.947	0.839	0.949	15
[#7][#6X3H0][#6X3H1]	0.935	0.774	0.851	31	0.968	0.903	0.941	15
[CH3]CC[OH]	0.953	0.667	0.811	18	0.905	0.571	0.906	15
[#6]1[#6][#6][#6][#6][#6]1	0.958	0.842	0.904	31	0.916	0.692	0.787	14
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.939	0.822	0.927	42	0.937	0.700	0.852	13
[CX4H3][CX4H2]	1.000	1.000	1.000	32	0.989	0.960	1.000	13
O=[#6][#6][#6X3]	0.935	0.731	0.812	28	0.926	0.696	0.713	13
[#7][#6H2][#6H2]	0.986	0.927	0.968	20	0.989	0.960	1.000	13
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.911	0.708	0.765	33	0.874	0.571	0.681	12
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.930	0.746	0.907	35	0.968	0.842	0.894	11
[CX4H2]([CX4H2])[CX3H0]	0.986	0.954	0.984	33	0.958	0.800	0.929	11
[#8][#6][#6][#8]	0.967	0.821	0.895	22	0.937	0.667	0.845	11
[#8][#6][#6]=[#8]	0.967	0.811	0.875	20	0.937	0.667	0.731	11
[CX4H3][CX3]	1.000	1.000	1.000	17	0.979	0.909	0.985	11
[CX4H3][CX3H0]	0.991	0.933	1.000	16	0.979	0.917	0.992	11
[CH2X4](O)[CX4H2]	0.991	0.909	0.934	12	0.989	0.957	0.983	11
[CX4H3][CX4H1]	0.981	0.943	0.989	34	0.979	0.900	0.955	10
O=[CX3H0][CX4H2][CX4H2]	0.986	0.954	0.982	33	0.968	0.824	0.899	10
[#7H2][#6H0]	0.907	0.444	0.623	24	0.916	0.500	0.645	10
[CH3][#6][#8]	0.991	0.944	0.991	18	0.979	0.900	0.947	10
[#7][#6][#7]	0.963	0.667	0.960	16	0.947	0.667	0.891	10
[CX4H2]([CX4H2])[CX4H1]	0.977	0.878	0.881	21	0.937	0.727	0.863	9
[CX4H2][CX4H2][CX4H2][CX4H2]	0.986	0.919	0.985	19	0.958	0.714	0.899	9
[#6X3][#7X3][#6X3]	0.925	0.429	0.499	18	0.916	0.600	0.610	9
[CX4H3][CX4]O	0.991	0.941	0.990	17	0.979	0.889	0.988	9
[#8][#6][#6][#6][#6]=[#8]	0.958	0.526	0.780	13	0.926	0.364	0.785	9
[CX4H3][CX4H0]	0.991	0.909	0.985	11	1.000	1.000	1.000	9
[CX4H]O	0.981	0.931	0.976	30	0.979	0.875	0.915	8
[#6]1[#6][#6][#6][#6][#7]1	0.963	0.778	0.862	20	0.926	0.462	0.780	8
[#7H2][#6H2]	0.981	0.875	0.954	17	0.979	0.875	0.985	8
[#6H3][#7]	0.991	0.929	0.955	15	0.979	0.857	0.940	8
[#7X3][#6H3]	0.995	0.963	1.000	14	0.979	0.857	0.935	8
[#7][#6H0][#7]	0.967	0.696	0.905	14	0.947	0.545	0.864	8
[#8][#6][#6][#6][#6][#8]	0.953	0.500	0.569	13	0.905	0.000	0.323	8
[#7][#6][#6][#6][#7]	0.967	0.533	0.735	11	0.937	0.500	0.686	8

[OX1H0]=[CX3H0][CX4H3]	1.000	1.000	1.000	11	0.968	0.800	0.969	8
[cX3H1]([nX2H0])[cX3H1]	0.991	0.909	0.925	11	0.947	0.545	0.817	8
[#7][#6][#6][#7]	0.986	0.800	0.931	9	0.937	0.500	0.557	8
[CX4H2]([OX2H1])[CX4H2]	0.995	0.909	0.874	6	1.000	1.000	1.000	8
[CH2X4](O)[CX4H2][CX4H2]	1.000	1.000	1.000	5	0.947	0.615	0.926	8
[CHX4]([CH3X4])[CH2X4]	0.981	0.895	0.986	19	0.968	0.769	0.844	7
CCCCC	0.967	0.800	0.843	19	0.947	0.545	0.827	7
[CHX3](=C)C	0.949	0.686	0.778	18	0.968	0.727	0.755	7
[CX4H3][cX3H0]	1.000	1.000	1.000	15	0.989	0.923	1.000	7
[#6H1][#7][#6H1]	0.981	0.750	0.871	10	0.926	0.364	0.681	7
[#6H1r5][#7]	0.972	0.571	0.896	10	0.968	0.727	0.827	7
[#7][#6][#6H3]	0.991	0.889	0.983	10	0.958	0.600	0.916	7
[CX4H2]([NX3H2])[CX4H2]	0.991	0.889	0.988	9	0.989	0.923	0.966	7
[#6H3][#6][#6][#6H3]	0.981	0.714	0.785	8	0.958	0.600	0.721	7
O[CX4H][CX4H2]	0.986	0.927	0.975	22	0.979	0.833	0.955	6
[OH][CX4H]	0.972	0.864	0.857	21	0.958	0.500	0.675	6
[#7H2][#6H1]	0.958	0.727	0.949	19	0.968	0.727	0.925	6
[#7H2][#6X4H1][#6X3]	0.981	0.875	0.984	18	0.979	0.800	0.899	6
[cH]cO	0.972	0.786	0.948	17	0.937	0.625	0.745	6
[#7H][#6X3H1]	0.944	0.143	0.476	11	0.926	0.000	0.362	6
[CX4H2]([NX3H1])[CX4H2]	0.986	0.800	0.856	9	0.968	0.667	0.862	6
[CX4H3][CX4H0][CX4H3]	1.000	1.000	1.000	7	0.979	0.800	0.913	6
[CX4H1]([CX4H3])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	0.937	0.000	0.858	6
[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	1.000	0.000	0.000	0	0.937	0.000	0.887	6
O=[#6][#6]=[#6X3]	0.972	0.824	0.952	17	0.989	0.889	0.938	5
[CX4H2]([CX4H3])[CX4H2]	0.991	0.938	0.993	16	0.989	0.909	0.963	5
[#8][#6][#6]=[#6X3]	0.981	0.867	0.937	16	0.979	0.750	0.805	5
[OX2H][cX3]:[c]	0.963	0.636	0.958	15	0.947	0.615	0.614	5
O=C[CX3H]	0.972	0.700	0.907	12	0.979	0.750	1.000	5
[#6]1[#6][#6][#6][#7]1	0.963	0.500	0.752	11	0.947	0.444	0.675	5
[#7X3H0]	0.981	0.800	0.868	11	0.968	0.667	0.558	5
[#6X4H3][#6][#8H]	0.986	0.842	0.980	10	0.989	0.909	1.000	5
[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.977	0.667	0.938	10	0.979	0.750	0.894	5
[#8]=[#6][#6][#6][#6]=[#8]	0.977	0.667	0.774	10	0.947	0.000	0.813	5
[#6H3][#7][#6H2]	0.986	0.769	0.959	7	0.968	0.571	1.000	5
[#6H2][#7][#6X3]	0.991	0.857	0.785	7	0.979	0.750	0.861	5
[OX1H0]=[CX3H0][CX4H0][CX4H3]	1.000	1.000	1.000	4	0.968	0.571	1.000	5
[#7][#6][#6][#6][#6][#7]	0.986	0.400	0.615	4	0.937	0.000	0.425	5
[OX1H0]=[CX3H0]([#6])[CX4H2]	1.000	1.000	1.000	18	0.979	0.750	0.944	4
[CX4H](O)CO	0.972	0.769	0.881	14	0.979	0.667	0.852	4
[#6X4H2][#6H1][#8H]	0.986	0.897	0.969	14	0.968	0.400	0.835	4
[#8][#6H1][#6H1]	0.944	0.333	0.592	14	0.989	0.889	1.000	4
[#8X1]=[#6X3][#6H2][#6H0]	0.986	0.800	0.875	9	0.989	0.857	0.944	4
[cX3H0][cX3H1][cX3H1][cX3H0]	0.977	0.615	0.864	9	0.968	0.400	0.449	4
[#6H3][#7][#6X3]	0.995	0.941	1.000	9	0.968	0.571	0.747	4

[#6H3][#6X3H0][#6H2]	1.000	1.000	1.000	8	0.979	0.667	1.000	4
[CX4H3][NX3H0]	0.981	0.714	0.949	8	0.979	0.667	0.729	4
[#8H][#6X4H1][#6X3H0]	0.986	0.769	0.938	8	0.979	0.667	0.842	4
[cX3H1]([nX2H0])[cX3H0]	0.986	0.769	0.885	7	0.968	0.400	0.731	4
[#6H3][#6]=[#6X3]	1.000	1.000	1.000	6	1.000	1.000	1.000	4
[CX4H2]([CX4H3])[CX4H1]	0.991	0.833	0.858	6	0.979	0.750	0.811	4
[cX3H1]([cX3H0])[cX3H0]	0.972	0.000	0.382	6	0.958	0.000	0.578	4
o[cH]	0.977	0.000	0.798	5	0.968	0.400	0.767	4
[cX3H1]([oX2H0])[cX3H1]	0.991	0.750	0.812	5	1.000	1.000	1.000	4
[#6]1[#6][#7][#6][#7]1	0.981	0.000	0.871	4	0.968	0.400	0.641	4
[OX2H1][CX4H0][CX4H3]	1.000	1.000	1.000	2	1.000	1.000	1.000	4
[CX4H3][OX2H0]	0.991	0.952	0.990	20	0.979	0.500	0.711	3
[#8H][#6H2][#6H1]	0.986	0.870	0.955	12	0.979	0.500	1.000	3
[CHX3]=[CHX3]	0.972	0.700	0.766	12	0.989	0.800	0.699	3
[CX4H2](O)[CHX4]	0.977	0.706	0.927	11	0.989	0.800	0.850	3
[#8]=[#6][#6H1]=[#6H1]	0.972	0.625	0.824	10	0.979	0.500	0.903	3
[#6H1]([#6H2])[#6H2]	0.972	0.571	0.812	10	0.979	0.500	0.492	3
[CX4H2]([OX2H1])[CX4H1]	0.991	0.889	0.957	10	0.979	0.667	0.514	3
[#8][#6][#6H2][#8]	0.991	0.875	0.959	9	1.000	1.000	1.000	3
[CX3H1](=[CX3H1])[CX3H0]	0.977	0.615	0.662	9	0.979	0.500	0.589	3
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.986	0.842	0.899	9	1.000	1.000	1.000	3
[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.981	0.714	0.849	9	0.979	0.500	0.733	3
[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	1.000	1.000	1.000	8	0.989	0.800	1.000	3
[#6X3][#6H2][#8]	0.995	0.933	1.000	8	1.000	1.000	1.000	3
[CX4H2]([OX2H0])[CX4H2]	0.995	0.923	1.000	7	0.989	0.857	1.000	3
[#6X3H2]	0.995	0.909	1.000	6	0.979	0.667	0.903	3
[cX3H1]([nX3H1])[cX3H1]	0.977	0.286	0.441	6	0.968	0.000	0.200	3
[CH2X3](=C)	0.995	0.909	1.000	6	0.979	0.667	0.711	3
[#6X3][#6X3]=[#6X3][#6X3]	0.977	0.286	0.522	6	0.968	0.000	0.168	3
[CX4H3][NX3H1]	0.991	0.750	0.827	5	0.968	0.000	0.903	3
[#8][#6H][#6X3][#6X3H]	0.977	0.000	0.781	5	0.968	0.000	0.764	3
[#6H2][#7][#6H2]	0.986	0.667	0.798	5	0.968	0.000	0.764	3
[OX2H1][CX4H2][#6X3H0]	0.991	0.667	0.852	4	0.989	0.800	1.000	3
[OX2H0][CX4H2][CX4H2][CX4H2]	1.000	1.000	1.000	4	0.989	0.800	1.000	3
[#8]=[#6X3][#6X3]=[#6X3][#6H3]	1.000	1.000	1.000	4	1.000	1.000	1.000	3
[#6X3][#6]=[#6][#6H3]	0.995	0.889	0.944	4	0.979	0.500	1.000	3
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.981	0.000	0.707	4	0.979	0.500	0.519	3
[CX4H2]([OX2H1])[cX3H0]	0.995	0.800	1.000	3	1.000	1.000	1.000	3
[#7][#6H1][#7]	0.995	0.667	1.000	2	0.979	0.500	0.850	3
[#6H0]([#6H3])([#6H3])[#8]	1.000	1.000	1.000	2	0.989	0.800	0.903	3
[CHX4]([CH3X4])[CH3X4]	0.995	0.966	0.992	15	0.979	0.500	0.708	2
[#8]=[#6][#6H2][#6H1]	0.963	0.333	0.960	10	0.989	0.667	1.000	2
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.995	0.933	0.944	8	0.989	0.800	1.000	2
[CX4H2]([CX4H1])[CX3H0]	0.981	0.667	0.897	8	0.989	0.667	1.000	2
[#6X3][#6H2][#7]	0.991	0.857	1.000	8	0.979	0.000	1.000	2

[OX1H0]=[CX3H0][OX2H0][CX4H3]	1.000	1.000	1.000	8	0.968	0.000	0.140	2
[OX2H0][CX3H0][CX4H2]	0.991	0.857	0.985	8	0.958	0.333	0.663	2
[#6X3][#6H2][#6X3]	0.995	0.933	0.985	8	0.979	0.500	0.184	2
[CX4H2][CX3]=C	1.000	1.000	1.000	8	0.989	0.800	1.000	2
O=[CX3H0][CX4H2][CX4H1]	0.977	0.545	0.969	8	0.989	0.667	1.000	2
O=[cX3]	0.977	0.444	0.750	7	0.968	0.000	0.223	2
[#6H1][#6H2][#6][#6][#7]	0.986	0.667	0.974	6	0.968	0.400	0.708	2
[#8]=[#6][#6]=[#8]	0.991	0.800	0.863	6	1.000	1.000	1.000	2
[#7][#6H2][#6H1]	0.977	0.444	0.669	6	1.000	1.000	1.000	2
[OX2H0][CX4H1][CX4H2][CX4H2]	0.986	0.667	1.000	6	0.989	0.667	1.000	2
O=CC=O	0.995	0.909	0.878	6	1.000	1.000	1.000	2
[cX3H1]([nX3H1])[cX3H0]	0.977	0.000	0.657	5	0.979	0.000	0.109	2
[OX1H0]=[CX3H0][CX4H2][CX3H0]	1.000	1.000	1.000	5	0.989	0.667	0.633	2
[OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]	0.995	0.889	0.963	5	0.989	0.667	1.000	2
[CX4H2]([CX3H0])[CX3H0]	1.000	1.000	1.000	5	0.989	0.667	0.792	2
[CX4H1]([OX2H1])([CX4H2])[CX3H0]	0.991	0.750	0.878	5	1.000	1.000	1.000	2
[#8][#6X3][#6X3]=[#6X3][#6H3]	1.000	1.000	1.000	4	1.000	1.000	1.000	2
[#6H2][#8][#6H1]	1.000	1.000	1.000	4	0.989	0.667	1.000	2
[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.986	0.571	0.811	4	0.989	0.667	1.000	2
[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.981	0.000	0.527	4	0.979	0.000	0.578	2
[#6X3H1]=[#6X3H0]	1.000	1.000	1.000	4	0.989	0.667	0.613	2
[CX4H2]([NX3H0])[CX4H2]	0.995	0.800	1.000	3	0.979	0.000	0.792	2
[CX3H2]=[CX3H1]	1.000	1.000	1.000	3	1.000	1.000	1.000	2
[CX4H3][CX3H0][CX3]=O	1.000	1.000	1.000	3	1.000	1.000	1.000	2
[#8][#6H2][#6H][#6X3]	0.995	0.800	1.000	3	0.979	0.000	1.000	2
[CX4H1]([NX3H1])([CX4H2])[CX3H0]	0.991	0.500	1.000	3	0.979	0.000	0.333	2
[#7H1][#6X4H1][#6X3]	0.986	0.000	0.903	3	0.979	0.000	0.417	2
[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.995	0.800	1.000	3	1.000	1.000	1.000	2
C1OCCC1	0.991	0.500	1.000	3	0.989	0.667	1.000	2
[CX4H2]([CX4H3])[CX4H0]	1.000	1.000	1.000	2	0.989	0.800	0.792	2
[#6H3][#6H0][#7H0][#6H0]	0.995	0.667	1.000	2	0.979	0.000	0.292	2
[#8][#6H2][#6H1][#6H0]	1.000	1.000	1.000	2	0.979	0.000	0.792	2
[OX2H1][CX4H0][CX4H2][CX4H3]	1.000	1.000	1.000	2	0.989	0.800	0.417	2
[CX4H3][CX4H0]([CX4H3])[OX2H0]	1.000	1.000	1.000	2	0.989	0.667	0.663	2
[cX3H0][cX3H1][cX3H0][OX2H1]	0.995	0.667	0.663	2	0.979	0.000	0.333	2
[#6H3][#7X3H0][#6X4H2][#6X4H2]	1.000	1.000	1.000	2	0.979	0.000	1.000	2
[#6X3]=[#6][#6][#6H3]	1.000	1.000	1.000	2	1.000	1.000	1.000	2
[#6H3][#6H0][#6H1][#7]	0.995	0.667	1.000	2	0.968	0.000	0.217	2
[OX1H0]=[CX3H0][CX4H2][CX4H0]	0.995	0.000	0.100	1	1.000	1.000	1.000	2
[CX4H2]([CX4H0])[CX3H0]	0.995	0.000	1.000	1	1.000	1.000	1.000	2
[OX1H0]=[CX3H0][CX3H1]=[CX3H0]	1.000	1.000	1.000	1	0.979	0.000	1.000	2
[CX3H1](=[CX3H0])[CX3H0]	1.000	1.000	1.000	1	0.979	0.000	1.000	2
[\$([CX2]#C)]	1.000	1.000	1.000	1	1.000	1.000	1.000	2
[CX2H1]#[CX2H0]	1.000	0.000	0.000	0	0.989	0.667	1.000	2
[#6H2][#6][#6X2]	1.000	0.000	0.000	0	0.979	0.000	1.000	2

[#8X2H0][#6X3H1][#6X3H1][#6X3H0]	1.000	0.000	0.000	0	0.979	0.000	0.633	2
[#8]=[#6][#6H1][#6H1]	0.967	0.632	0.659	12	0.958	0.000	0.029	1
[CX4H2][CX3H]	0.977	0.667	0.784	10	1.000	1.000	1.000	1
[CX4H3][CX4H1][OX2H1]	0.995	0.933	1.000	8	1.000	1.000	1.000	1
[NH1][#6][#7]	0.986	0.727	1.000	7	0.989	0.000	1.000	1
[#6H3][#6H1][#6H1][#7]	0.972	0.250	0.617	7	0.989	0.000	1.000	1
[CX4H2]([CX4H2])[CX3H1]	0.986	0.667	0.754	6	1.000	1.000	1.000	1
[CX4H2]([CX4H3])[CX3H0]	1.000	1.000	1.000	5	1.000	1.000	1.000	1
[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.995	0.889	1.000	5	0.989	0.000	0.250	1
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	1.000	1.000	1.000	5	1.000	1.000	1.000	1
[#7][#6]([#7])=[#7]	0.991	0.750	1.000	5	0.989	0.000	0.083	1
[#8][#6][#6]=[#6][#6][#8]	0.977	0.000	0.938	5	0.989	0.000	0.083	1
[#6H2][#6X3H0][#6H2]	1.000	1.000	1.000	5	1.000	1.000	1.000	1
[NH1]=[#6][#7]	1.000	1.000	1.000	5	0.979	0.000	0.100	1
[#8]=[#6][#6]=[#6][#6]=[#8]	0.986	0.571	0.918	5	0.989	0.000	1.000	1
[#6]=[#7H]	0.995	0.889	1.000	5	0.979	0.000	0.083	1
[#7][#6H0]=[#7]	1.000	1.000	1.000	5	0.979	0.000	0.083	1
[#7][#6]=[#7]	1.000	1.000	1.000	5	0.979	0.000	0.071	1
[#6]#[#7]	1.000	1.000	1.000	4	1.000	1.000	1.000	1
[CX4H2]([OX2H0])[CX4H3]	1.000	1.000	1.000	4	1.000	1.000	1.000	1
[#8][#6][#6]=[#6][#6]=[#8]	0.981	0.000	0.811	4	0.989	0.000	1.000	1
[#7][#6H1][#6H2r5]	0.995	0.857	1.000	4	0.989	0.667	0.250	1
[OX1H0]=[CX3H0][CX4H2][CX4H3]	1.000	1.000	1.000	4	1.000	1.000	1.000	1
[CX4]([CX4H3])([CX4H3])[CX4H3]	1.000	1.000	1.000	4	0.989	0.667	0.250	1
[CX4H2]([NX3H2])[CX4H1]	0.995	0.800	0.817	3	0.989	0.000	1.000	1
[CX4H2]([NX3H1])[CX4H1]	0.986	0.000	0.314	3	0.989	0.000	0.071	1
[CX4H2]([NX3H0])[CX3H0]	1.000	1.000	1.000	3	0.989	0.000	1.000	1
[CX4H1]([OX2H0])([CX4H2])[CX4H2]	1.000	1.000	1.000	3	0.989	0.000	1.000	1
[#7H1]=[#6H0][#7X3][#6H3]	1.000	1.000	1.000	3	0.989	0.000	1.000	1
[#7][#6H2][#6H2][#7]	1.000	1.000	1.000	3	0.979	0.000	0.100	1
[CX3H2]=[CX3H0]	0.995	0.800	1.000	3	0.979	0.000	0.167	1
[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.991	0.500	1.000	3	0.989	0.000	1.000	1
[CX3H2]=[CX3H0]([#6])[#6]	0.995	0.800	1.000	3	0.989	0.000	1.000	1
[CX4H3][CX3H1]	1.000	1.000	1.000	3	1.000	1.000	1.000	1
[CX4H1]([CX4H3])([CX4H3])[CX4H1]	1.000	1.000	1.000	2	0.989	0.000	1.000	1
[#6X3H1]=[#6X3H1][#6X3H0][#6X3H1]	0.991	0.000	0.333	2	0.989	0.000	0.036	1
[CX4H1]([OX2H1])([CX4H3])[CX3H0]	1.000	1.000	1.000	2	1.000	1.000	1.000	1
[#6X3][#6X3][#6X3]=[#6X3]	0.995	0.667	0.663	2	0.989	0.000	0.045	1
[#6X3H1][#7X3H0]	0.995	0.667	1.000	2	1.000	1.000	1.000	1
[CX3H0](=[OX1H0])([OX2H0])[CX3H1]	0.995	0.667	1.000	2	0.989	0.000	0.250	1
[OX2H1][CX4H2][#6X3H0][#8X2H0]	0.995	0.667	1.000	2	1.000	1.000	1.000	1
[CX3H0](=[CX3H1])([CX4H3])[CX3H0]	1.000	1.000	1.000	2	0.979	0.000	0.250	1
[#6H2][#6X3H0]=[#6H2]	1.000	1.000	1.000	2	0.989	0.000	1.000	1
[#6H2][#6X2]	0.995	0.667	1.000	2	1.000	1.000	1.000	1
[OX2H0][CX4H1][CX4H3]	1.000	1.000	1.000	2	1.000	1.000	1.000	1

[CX4H1]([OX2H0])([CX4H3])[CX4H2]	1.000	1.000	1.000	2	1.000	1.000	1.000	1
[#8]1[#6][#6][#6][#6]1	0.995	0.667	1.000	2	0.979	0.000	0.050	1
[CX3H1](=[CX3H1])[cX3H0]	0.995	0.000	1.000	1	0.989	0.000	0.045	1
[CX3H0](=[OX1H0])([NX3H0])[CX4H2]	0.995	0.000	0.125	1	0.989	0.000	0.100	1
[cX3H1]([nX3H0])[cX3H1]	0.995	0.000	0.167	1	1.000	1.000	1.000	1
[#7][#7]	0.995	0.000	0.063	1	0.979	0.000	0.125	1
[#7][#7H1]	0.995	0.000	0.071	1	0.989	0.000	0.056	1
[OX2H1][CX4H0][CX4H2][CX3H0]	0.995	0.000	0.125	1	0.989	0.000	1.000	1
[CX4H3][nX3H0]	1.000	1.000	1.000	1	1.000	1.000	1.000	1
[CX4H2]([OX2H0])[CX4H1]	1.000	1.000	1.000	1	0.989	0.000	1.000	1
[CX3H0](=[OX1H0])([OX2H0])[CX4H3]	1.000	1.000	1.000	1	0.989	0.000	0.125	1
[CX4H3][CX3H0]=[CX3H2]	0.995	0.000	1.000	1	0.979	0.500	0.167	1
[CX3H1](=[CX3H1])[CX3H1]	0.995	0.000	0.125	1	0.989	0.000	0.250	1
[#7][#6H2][#6H2][#6H1]	0.995	0.000	1.000	1	1.000	1.000	1.000	1
[CX3H0](=[OX1H0])([CX4H1])[CX3H0]	1.000	1.000	1.000	1	1.000	1.000	1.000	1
[#6H][#8][#6H]	1.000	1.000	1.000	1	1.000	1.000	1.000	1
[OX2H0][CX3H0][CX4H3]	1.000	1.000	1.000	1	0.989	0.000	0.250	1
[OX2H0][CX4H2][CX4H1][CX4H2]	1.000	1.000	1.000	1	0.989	0.000	0.250	1
[#7][#6][#6]=[#6X3]	1.000	1.000	1.000	1	0.989	0.000	0.056	1
[CX3H1](=[CX3H1])[CX4H3]	0.995	0.667	1.000	1	0.989	0.000	1.000	1
[#8][#6X3][#6X3][#6X3][#6H3]	1.000	1.000	1.000	1	0.989	0.000	1.000	1
[CX4H2]([NX3H1])[CX3H0]	1.000	1.000	1.000	1	0.989	0.000	1.000	1
[CX3H0](=[OX1H0])([NX3H1])[CX4H1]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
CC=CC=CC	1.000	0.000	0.000	0	0.989	0.000	0.100	1
[CX2H0](#[NX1H0])[CX4H1]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[#6H2][#6][#6X2]	1.000	0.000	0.000	0	1.000	1.000	1.000	1
[CX2H0](#[CX2H1])[CX4H0]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[CX4H2]([CX4H2])[CX2H0]	1.000	0.000	0.000	0	1.000	1.000	1.000	1
[#6]1[#8][#6][#8][#6]1	1.000	0.000	0.000	0	1.000	1.000	1.000	1
[#8]=[#6][#6H0][#6]=[#8]	1.000	0.000	0.000	0	0.989	0.000	0.100	1
[#7][#6]=[#6X3]	1.000	0.000	0.000	0	0.989	0.000	0.083	1
[CX4H1]([CX4H2])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	0.989	0.000	0.250	1
[OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX4H2]	1.000	0.000	0.000	0	0.989	0.000	0.125	1
[#6H3][#6H1r5]	1.000	0.000	0.000	0	0.989	0.000	0.167	1
[#7][#6H0][#6H1]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[CX3H1](=[CX3H2])[CX4H0]	1.000	0.000	0.000	0	1.000	1.000	1.000	1
[CX2H0](#[CX2H1])[CX4H2]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[#6X2][#6X4H1]	1.000	0.000	0.000	0	0.989	0.000	0.250	1
[#6H3][#6H0][#7][#6H3]	1.000	0.000	0.000	0	0.989	0.000	0.250	1
[#7][#6X3H0]=[#6X3H1]	1.000	0.000	0.000	0	0.989	0.000	0.250	1
[#7][#6]=[#6][#6X3]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[CX3H2]=[CX3H1][CX4H0][OX2H1]	1.000	0.000	0.000	0	1.000	1.000	1.000	1
[CX3H0](=[OX1H0])([CX4H3])[CX3H0]	1.000	0.000	0.000	0	1.000	1.000	1.000	1
[CX3H1](=[CX3H2])[CX4H2]	1.000	0.000	0.000	0	0.989	0.000	1.000	1

[CX3H0](=[OX1H0])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[cX3H1]([OX2H0])[cX3H0]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[#6X3]=[#6X3][#6X3]=[#6X3]	1.000	0.000	0.000	0	0.989	0.000	0.125	1
[#6H3][#6H2][#6H1][#7]	1.000	0.000	0.000	0	0.989	0.000	1.000	1
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.995	0.941	0.988	9	1.000	0.000	0.000	0
[CX3H1](=[O])[#6]	1.000	1.000	1.000	8	1.000	0.000	0.000	0
[OX1H0]=[cX3H0][cX3H1]	0.977	0.286	0.639	5	0.989	0.000	0.000	0
[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.981	0.333	0.693	5	1.000	0.000	0.000	0
[CX4H2]([CH])[CH]	0.991	0.750	0.865	5	0.989	0.000	0.000	0
[NH1][#6]=[#7]	1.000	1.000	1.000	5	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[CX4H2]	1.000	1.000	1.000	5	1.000	0.000	0.000	0
[OX2H1][CX4H1][CX4H1][OX2H1]	1.000	1.000	1.000	5	1.000	0.000	0.000	0
[CX4H2]([CX4H1])[CX4H1]	0.995	0.857	1.000	4	0.989	0.000	0.000	0
[CX3H1](=[OX1H0])[CX4H2]	0.986	0.400	0.820	4	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H2])[CX3H0]	1.000	1.000	1.000	4	0.989	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.991	0.667	0.871	4	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.995	0.857	1.000	4	0.989	0.000	0.000	0
O[CX4H]([CX4H2])[CX4H1]	0.991	0.667	0.871	4	0.989	0.000	0.000	0
[CX4H3][OX2H0][CX4H2]	0.995	0.857	0.944	4	1.000	0.000	0.000	0
[OX2H0][CX4H1][OX2H0]	1.000	1.000	1.000	4	0.989	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.995	0.857	1.000	4	1.000	0.000	0.000	0
[#8][#6H2][#6H0][#6H2][#8]	0.991	0.500	1.000	3	1.000	0.000	0.000	0
[#8]=[#6][#6H2][#8]	0.995	0.800	1.000	3	0.989	0.000	0.000	0
[#7][#6][#6][#6X3]	1.000	1.000	1.000	3	1.000	0.000	0.000	0
[#7H1][#6H0][#7X3][#6H3]	0.991	0.667	0.903	3	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX4H2][CX4H2]	0.991	0.500	0.433	3	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H2])[CX4H1]	0.986	0.000	0.405	3	1.000	0.000	0.000	0
[#6H3][#6H0]([#6H2])[#6H2]	0.986	0.000	0.406	3	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX3H0]	0.995	0.800	1.000	3	0.989	0.000	0.000	0
[CX4H2]([OX2H1])[CX4H0]	0.995	0.800	1.000	3	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX3]=O	0.995	0.800	1.000	3	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([OX2H0])[CX4H2]	1.000	1.000	1.000	3	1.000	0.000	0.000	0
[#8]=[#6H][#6X3][#6X3H]	0.995	0.800	1.000	3	1.000	0.000	0.000	0
CCCC=C	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[OX2H0][CX4H2][#6H0]	0.995	0.667	1.000	2	1.000	0.000	0.000	0
[CX4H2]([CX4H2])[cX3H0]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX2H0][CX4H2][#6X3H0]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H2]([OX2H1])[CX3H1]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[#8][#6H2][#6H]=[#6X3]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[#6X4H1][#6X4H1][#6X4H1]	0.991	0.000	0.217	2	1.000	0.000	0.000	0
CCCC=CC	1.000	1.000	1.000	2	1.000	0.000	0.000	0
O[CX4H2][CX3H1]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H2])[CX4H2]	0.991	0.000	1.000	2	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([OX2H0])[CX3H0]	0.995	0.667	1.000	2	1.000	0.000	0.000	0
[CX4H2]([NX3H2])[CX3H0]	0.995	0.667	0.663	2	1.000	0.000	0.000	0

[CX3H](O)	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H3])[CX4H3]	1.000	1.000	1.000	2	0.989	0.000	0.000	0
[#6H1][#6H2][#6H2][#6H1]	0.995	0.667	1.000	2	1.000	0.000	0.000	0
[#8][#6H1][#6H1][#6H3]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.986	0.000	0.417	2	1.000	0.000	0.000	0
O=[#6][#6H][#6H0]	0.991	0.000	1.000	2	1.000	0.000	0.000	0
[CX2H0](#[NX1H0])[CX4H2]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[CX4H3]	1.000	1.000	1.000	2	0.989	0.000	0.000	0
O[CX4H2][CX4H2]O	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H2]([OX2H0])[CX3H0]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[#6H3][#6]=[#6][#6H3]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H3])[CX4H2]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H3][CX3H0][CX4H3]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[#6H2][#6H1][#6H1][#6H2]	0.991	0.000	0.155	2	1.000	0.000	0.000	0
[CX4H1][CX4H2][CX4H2][CX4H1]	0.991	0.000	1.000	2	1.000	0.000	0.000	0
[CX4H2][OX2H0][CX4H2]	0.991	0.500	0.792	2	1.000	0.000	0.000	0
O=C[CH2][CH2]O	0.995	0.667	1.000	2	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H2])[CX3H0]	0.995	0.667	1.000	2	1.000	0.000	0.000	0
[CX3H]O[CX4H2]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H2][OX2H0]	1.000	1.000	1.000	2	1.000	0.000	0.000	0
[CX4H](O)([CH])[CH]	0.991	0.000	0.292	2	1.000	0.000	0.000	0
[#6H2][#6H1]=[#6H1][#6H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX4H2]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[#8][#6H2][#6H1]=[#6H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6H2r3]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H3])[CX3H0]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1]1	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[#7][#6][#6X3]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6H3][#8][#6H0][#8]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([OX2H0])[CX4H1]	0.995	0.000	0.125	1	1.000	0.000	0.000	0
C1CCC1	1.000	1.000	1.000	1	0.989	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H2])[CX4H2]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX4H2][CX4H1]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX3H1]=[CX3H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6H2][#6H1r3]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H2][CX3H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
O=C[CH2][CX3H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX2H0](#[NX1H0])[CX4H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[OX2H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[NX3H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H2]([CX4H2])[CX4H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
CC=CCC=C	1.000	1.000	1.000	1	1.000	0.000	0.000	0

[CX4H2]([CX3H0])[CX2H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H2]([OX2H1])[CX3H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#8]=[#6][#6H2][#6X2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H3][cX3H0][oX2H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
CCC=CCC	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H][CX4H]	1.000	1.000	1.000	1	0.989	0.000	0.000	0
C1OC1	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6X3H1][#6H1][#6H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX3H0][CX4H3]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX2H1][CX4H2][CX3H0][CX4H2]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H2][CX4H2]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[OX2H0][CX3H1]=[CX3H1][CX4H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[cX3H0]([cX3H1])([cX3H0])[CX4H2]	0.995	0.000	0.167	1	1.000	0.000	0.000	0
[#8X2H0][#6X3H0][CX4H2][CX4H1]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[#8][#6]=[#6H2]	1.000	1.000	1.000	1	0.989	0.000	0.000	0
[CX3H2]=CO	1.000	1.000	1.000	1	0.989	0.000	0.000	0
[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H2]([CX3H1])[CX3H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H2]([NX3H2])[CX4H0]	0.995	0.000	0.250	1	1.000	0.000	0.000	0
[O][CX3H1]=[CX3H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#8]1[#6][#6][#6][#6]=[#6]1	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#8]=[#6H1][#7]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H1]1[CX4H2][CX4H2][CX4H2]1	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H2]([CX4H1])[CX3H1]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[CX4H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#8]=[#6H][#6X3]=[#6X3H]	0.995	0.000	0.167	1	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[CX3H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[CX3H1]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[OX2H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#8]=[#6H1][#6H1]	0.995	0.000	0.167	1	1.000	0.000	0.000	0
[#6]1[#6]=[#6][#6][#6]=[#6]1	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX2H1][CX4H1]([#6X3H0])[CX4H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6]1[#6][#7][#6][#6][#7]1	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#8][#6H2][#6X3H]=[#6X3H]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1]1[CX4H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H2])[CX3H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H1])[CX3H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6H2][#6H1][#6H1]=[#6H2]	1.000	1.000	1.000	1	0.989	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H3])[CX4H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX2H0]([#CX2H0])[CX3H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H2])[CX4H1]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H2])[CX4H2]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[CX4H1]	1.000	1.000	1.000	1	0.989	0.000	0.000	0
[CX4H3][CX2H0]	1.000	1.000	1.000	1	1.000	0.000	0.000	0
[#6X3][#6][#6][#6H3]	1.000	1.000	1.000	1	1.000	0.000	0.000	0

[CX4H1]([CX4H2])([CX3H0])[CX3H0]	0.995	0.000	1.000	1	1.000	0.000	0.000	0
[#6H3][#8][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([OX2H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H3])([CX4H3])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1]1[CX4H2][CX4H0]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H2][#6H2][#6X2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]1[CX4H2][CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX4H2][CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6]=[#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX3H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H0][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[NX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H2])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#7][#6H0][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H2][CX4H0]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2][#6X3H0][#6X3H1][#8X2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H3])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0]#[CX2H1][cX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0]#[CX2H1][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[NX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1][CX4H1]([CX4H1])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H2])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([OX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([NX3H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX3H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#8][#6][#6]1=[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX4H1]([CX4H1])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[cX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]=[#6H1][#6H0][#6]=[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[CX4H2]([CX4H3])[cX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H2])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C=CC=CC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCC#CC=C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([OX2H0])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([NX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[cX3H0]([oX2H0])([cX3H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H2])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([OX2H0])[cX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H2])([CX4H2])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([CX4H3])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H0]([CX4H3])[CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[cX3H0]([oX2H0])([cX3H0])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]=[#6X3][#6X3][#6X3][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H3])([CX4H3])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H2])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#7]=[#6H0][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX3H1]=[CX3H1][CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H2])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1][CX4H2r0][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1][CX4H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[oX2H0][cX3H0][cX3H0][CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2][#7]=[#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#7][#6]=[#7]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6]=[#6][#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[NH1][#6H1][#6H1][NH1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1][#7]=[#6H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H0])([NX3H1])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[NX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6H1]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3][#7]=[#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[NX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[NX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[#7][#6][#6]=[#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6]=[#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6X3H0][#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6][#6]=[#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6][#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#7][#6X4H1][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#7][#6][#6][#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[NX1H0])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([NX3H2])([CX4H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[NX1H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]#[#6][#6]=[#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2][#7]=[#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1r5]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[NX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2][#7][#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1][#7H1][#6H2r4]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1][#6H2][#6H0][#6H1][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6][#6][#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6][#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H0])([NX3H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[NX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][NX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#7]=[#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#7X2]=[#6H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#7][#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6H1][#6X2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1][#6H2][#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7H]=[#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[CX3H1](=[NX2H1])[NX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([NX3H2])([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H1])([NX3H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H3])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1r4][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H3])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H1])[NX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H0])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H1][#6H2][#6][#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#6H1][#7][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H1])([NX3H1])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#7][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6][#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2][#7][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[cX3H1]([nX3H0])[nX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6]=[#6][#6][#7]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H0])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H0])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6]=[#6][#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[cX3H0]([nX2H0])([cX3H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6]=[#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H1]=[#6X3H0][#6X4H1][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#7]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#6H0][#6H1]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6H0][#6H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#7H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6H1r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#7]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6]=[#6][#6][#7]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H0])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[#6H3][#6H1][#6H1]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[NX2H1])([NX3H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[NX2H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2]=[#7][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[NX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H2])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#7]=[#6]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6][#6][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H1][#6X3H0][#6X4H1][#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H1])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6][#6][#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([NX3H1])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7]=[#6][#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7][#6]=[#6][#6][#6]=[#7]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6]=[#6][#7]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[cX3H1]([nX3H0])[cX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#7X2]=[#6X3H1][#7X3H0][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([NX3H0])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H2])([CX4H2])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H1][#8][#6H2][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H0])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H2])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H1][#CX2H0][CX4H1][OX2H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H2])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H]=[#6X3][#6X3H]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][CX3H1]=[CX3H0][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX3H1]=[CX3H1][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O[CX3H]=[CH0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2][OX2H0][CX3H1]=[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2][#6X3H0]=[#6X3H1][#8X2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#6][#6][#6][#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]1[CX4H0][CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H2])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H0]([CX4H2])[CX4H2][CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2r3][CX4H0r3][OX2H0r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1]1[CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]1[CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX3H1]=[CX3H1][CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[CX4H0]([OX2H0])([CX4H3])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([OX2H0])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6]=[#6][#6X3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1CCCC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]1[#6][#6]=[#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([OX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H2][CX3H0]=[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([OX2H0])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[CX2H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#6][#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H2]=[#6X3][#6X3]=[#6X3H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O1CC=CC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H3])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0][CX4H2][CX3H1]=[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6X3]=[#6X3][#6X3][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([OX2H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H1])[CX3H0]	1.000	0.000	0.000	0	0.989	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H3]	1.000	0.000	0.000	0	0.989	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H2])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#6]1=[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2r3][CX4H2r3][CX4H0r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6]([#8])[#6]1[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C=CCCC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX3H0][CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([CX4H3])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[CX2H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H1][CX4H1]([CX4H1])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O[CH][CX3]=[CX3H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1COC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0r4][CX4H1r4][CX4H1r4]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX4H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6]([#6H3])[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][CX4H0r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX3H0]=[CX3H2]	1.000	0.000	0.000	0	0.989	0.000	0.000	0
C=CCCC=C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6]1[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX3H1]=[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCC=CC=C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([OX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1OCCCCC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O1CCC=C1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8X2H0][#6X3H0][CX4H2][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX4H2][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2r3][#6H2r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2]1[#6H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2r3][CX4H2r3][CX4H1r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H0]=[#6H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1r3][CX4H2r3][CX4H0r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([OX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1CC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCCC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H2][CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([OX2H0])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1r6][CX4H2r6][CX4H2r6][OX2H0r6]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0r6][CX4H2r6][OX2H0r6]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2]1[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H2][CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1CC1O	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[CX4H2]([OX2H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H2][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2r3][#6H0r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][OX2H0][CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1r3][CX4H2r3][CX4H1r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H0]([#6])([#6])[#6]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0]([#CX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1OCCCC=C1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H1][#6H2][#6H1][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0]([#CX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCC#CCC	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCCC#CC	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H3])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O[CH][CX2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CC#CCC=C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O[CX4H1][CX3H1]=[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX3H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#6]1[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H1][#6X4H][#8H]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1]1[CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1][CX4H1]([CX4H1])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6]=[#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H][#6X3]=[#6X3H]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C=CC=CC=C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H1][#6X3H1]=[#6X3H0][#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([OX2H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[OX1H0])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H][#6H2][#6H2][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([OX2H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O[CX4H1][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1][CX3H0]=[CX3H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[CX4H1]([CX4H3])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H1]([CX4H1])[OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1]1[CX4H1][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX4H1]([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1OC=CCCC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX3H0]=[CX3H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]=[#6H1][#6H1][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H3])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#8][#6][#6]1[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H2])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H0][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H3])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CC#CCC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H3])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX4H1]([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[CX2H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H3])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H0][CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCC=CC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H0][CX4H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1]1[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H3])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[#6X3H0][#6X3H0][#8X2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H2])([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H0])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]1[CX4H2][CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][OX2H0][CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H0][CX4H2][CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H2])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([OX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]1[CX4H2][CX4H1][CX4H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H1]([OX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1][CX4H1][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([OX2H0])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([OX2H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[CX3H0](=[CX3H1])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX3H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
O[CH]=[CH]O	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1][CX4H1][CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX4H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX4H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][OX2H0][CX4H2][CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1][CX4H1]([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X2][#6H1][#6X2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H1]([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6][#6][#6]=[#6][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[CX2H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X2][#6X3H]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX3H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H1]([OX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][OX2H0][CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([OX2H0])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#6H2][#6H1r4]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H1]=[#6H1][#6H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]1[#6][#6][#8][#6][#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1]([CX4H1])[CX4H2][CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CC=CC#CC	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX3H0]=[CX3H0][CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([OX2H0])[CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6H1][#6H2][#6H1]=[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0r5][CX4H2][OX2H0r5]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H3])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H2]=[#6][#6H2][#8H]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8X2H0][#6X3H0][CX4H2][CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX4H0][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][CX3H0][CX4H2][CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([OX2H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#8][#6X3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][OX2H0][CX3H1]=[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H1](=[CX3H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[#6X2][#6H2][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX2H0][CX2H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H2][CX4H1]([CX4H1])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6][#6][#6][#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]1[#6][#6][#6]=[#6][#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6]=[#6][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#6H1]([CH3])[#6][#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H3])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6]1[#8][#6][#6H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX4H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H1][CX4H2][CX4H1][CX4H2]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H2]=[#6][#6X2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X3H2]=[#6][#6H2][#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H2]=[CX3H0][CX4H2][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H2])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H1]([OX2H0])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1]1[CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CC=CCC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#6X3][#6X3]=[#6X3H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1OC([CX4H3])C1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H3])([CX4H3])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H3])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][OX2H0][CX3H1]=[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1r4][CX4H2r4][CX4H1r4]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H1][CX3H0]=[CX3H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[CX2H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([CX4H2])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([CX4H0])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H1])([CX4H2])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6]=[#6][#6][#6]=[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX2H0](#[CX2H0])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H1])([CX4H3])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H2])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

[OX2H0r0][CX4H2r0][OX2H0r0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX3H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8X2H0][#6X3H1]=[#6X3H1][#6X3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([OX2H0])([CX4H1])[CX4H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
CCC#CC#C	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6X2][#6X2]#[#6X2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0]1[CX4H1][CX4H2][CX4H1]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#6H1r3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H2]([OX2H1])[CX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H2])([CX3H1])[CX3H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[OX1H0])([CX4H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8][#6X4H0]([#6X3])([#6X3])	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#6H3][#6]([#6X3])([#6X3])[#8]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H1]([CX4H1])[CX4H1][CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX3H1])[CX3H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[#8]1[#6]=[#6][#6][#6]=[#6]1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([CX4H3])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H3][#6X3H0]=[#6X3H0][CX4H3]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX3H0](=[CX3H0])([OX2H0])[CX4H2]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[OX2H0][CX4H2][CX3H0][OX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[CX4H1]([CX4H1])([CX4H1])[CX4H1]	1.000	0.000	0.000	0	1.000	0.000	0.000	0
C1OCCC=CC1	1.000	0.000	0.000	0	1.000	0.000	0.000	0
[cX3H1]([oX2H0])[nX2H0]	1.000	0.000	0.000	0	1.000	0.000	0.000	0

4.2 Individual substructure results with SMART graphs

Top row: SMART string.

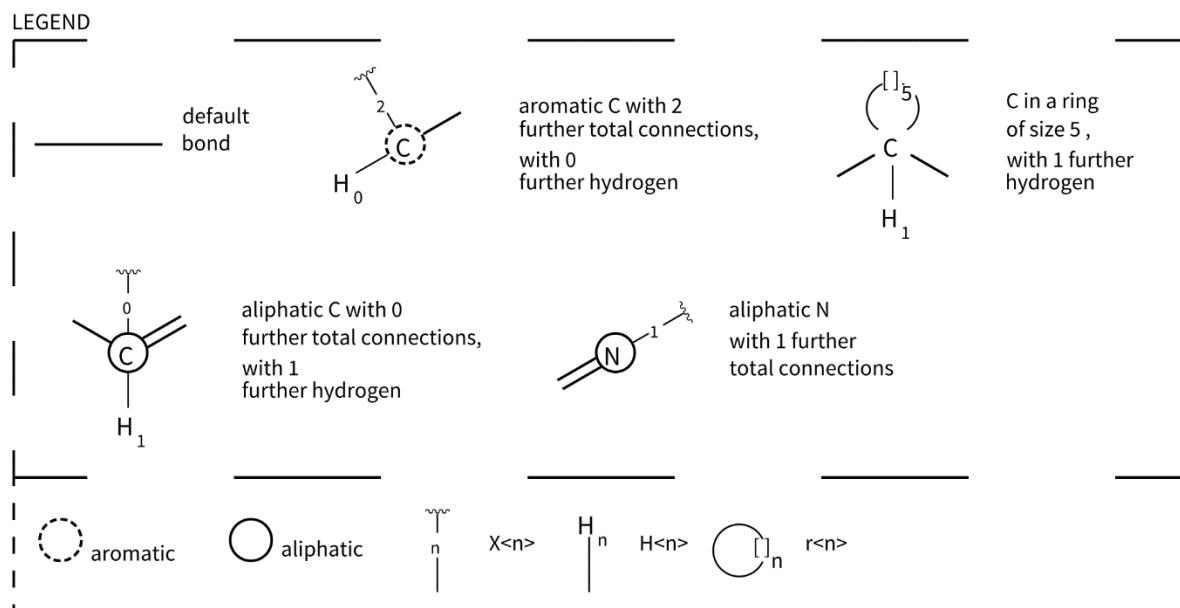
Middle row: validation accuracy, F₁ score, PRC-AUC score, support.

Bottom row: test accuracy, F₁ score, PRC-AUC score, support.

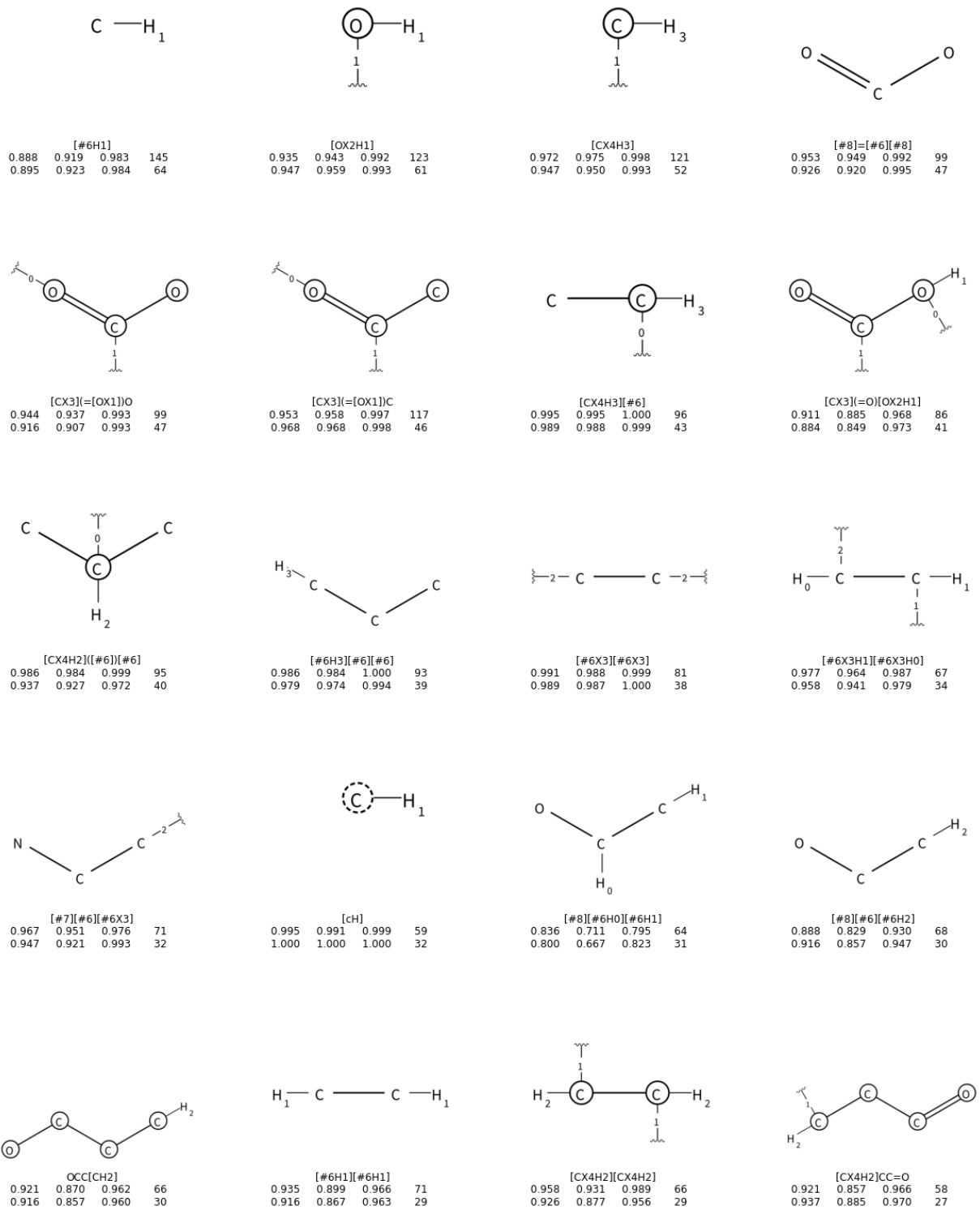
Sorted by number of supports in the test and validation set.

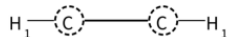
There are 214 examples in validation set and 95 examples in test set.

The SMART string visualization were generated using the SMARTSviewer [smartsview.zhb.uni-hamburg.de]. Copyright: ZBH – Center for Bioinformatics Hamburg.



Picture created by the SMARTSviewer [smartsview.zhb.uni-hamburg.de].
Copyright: ZBH - Center for Bioinformatics Hamburg.

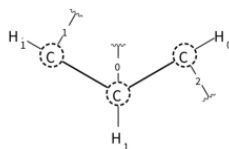




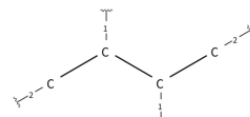
[cH][cH]
0.991 0.982 1.000 57
0.958 0.929 0.994 27



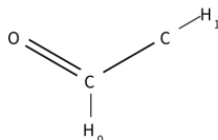
[#6H3][#6H0]
0.977 0.938 0.993 41
0.979 0.963 0.999 27



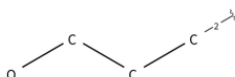
[cX3H1][cX3H1][cX3H0]
0.977 0.954 0.959 54
0.968 0.941 0.994 25



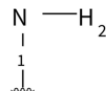
[#6X3][#6X3][#6X3][#6X3]
0.986 0.972 0.997 54
0.947 0.906 0.995 24



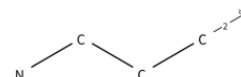
[#8]=[#6H0][#6H1]
0.907 0.792 0.921 51
0.884 0.732 0.925 24



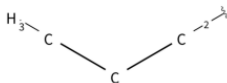
[#8][#6][#6][#6X3]
0.916 0.800 0.931 50
0.947 0.898 0.964 24



[#7X3H2]
0.949 0.893 0.964 55
0.905 0.816 0.862 23



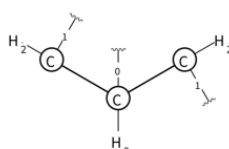
[#7][#6][#6][#6X3]
0.977 0.944 0.989 46
0.937 0.864 0.939 23



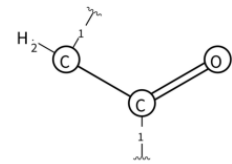
[#6H3][#6][#6X3]
0.977 0.933 0.991 37
0.905 0.791 0.857 23



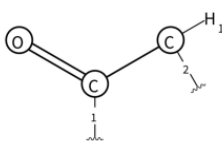
[#6H1][#6H2]
0.916 0.842 0.925 58
0.916 0.810 0.919 21



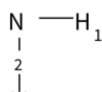
[CX4H2][CX4H2][CX4H2]
0.981 0.937 0.986 33
0.968 0.923 0.989 20



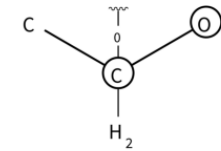
[CX4H2][CX3]=O
0.930 0.880 0.965 65
0.905 0.757 0.914 19



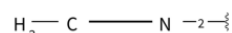
O=[CX3][CX4H]
0.953 0.857 0.955 35
0.968 0.914 0.952 19



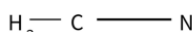
[#7X3H1]
0.864 0.453 0.604 32
0.779 0.222 0.490 19



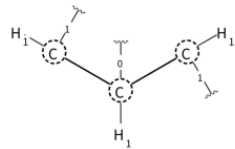
[CX4H2][#6][O]
0.967 0.904 0.981 36
0.979 0.944 0.988 18



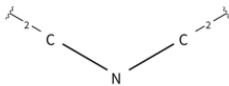
[#7X3][#6H2]
0.986 0.959 0.953 35
0.958 0.882 0.979 17



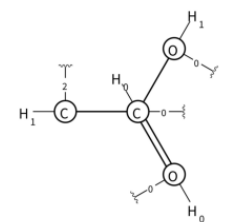
[#7][#6H2]
0.977 0.932 0.973 35
0.989 0.971 0.985 17



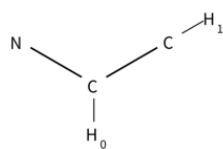
[cX3H1][cX3H1][cX3H1]
0.944 0.872 0.949 44
0.947 0.857 0.967 16



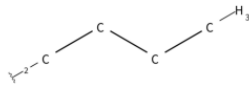
[#6X3][#7][#6X3]
0.939 0.800 0.846 34
0.905 0.727 0.860 16



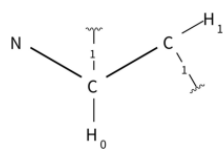
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.902 0.667 0.718 32
0.916 0.692 0.882 16



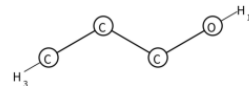
[#7][#6H0][#6H1]
0.930 0.754 0.841 31
0.958 0.875 0.931 16



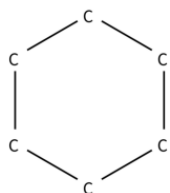
[#6X3][#6][#6H3]
0.925 0.800 0.915 42
0.947 0.839 0.949 15



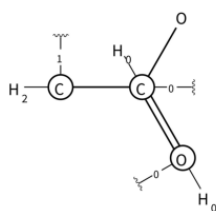
[#7][#6X3H0][#6X3H1]
0.935 0.774 0.851 31
0.968 0.903 0.941 15



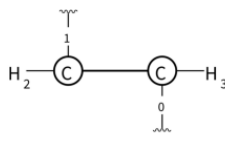
[CH3]CC[OH]
0.953 0.667 0.811 18
0.905 0.571 0.906 15



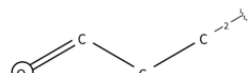
[#6]1[#6][#6][#6][#6]1
0.958 0.842 0.904 31
0.916 0.692 0.787 14



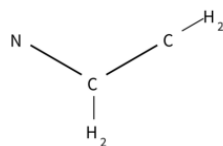
[OX1H0]=[CX3H0][#8][CX4H2]
0.939 0.822 0.927 42
0.937 0.700 0.852 13



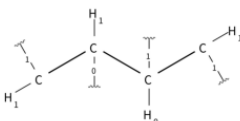
[CX4H3][CX4H2]
1.000 1.000 1.000 32
0.989 0.960 1.000 13



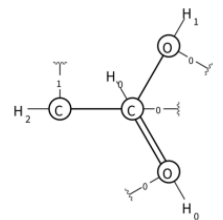
O=[#6][#6][#6X3]
0.935 0.731 0.812 28
0.926 0.696 0.713 13



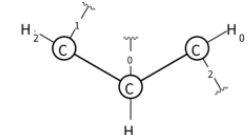
[#7][#6H2][#6H2]
0.986 0.927 0.968 20
0.989 0.960 1.000 13



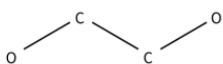
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.911 0.708 0.765 33
0.874 0.571 0.681 12



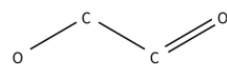
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.930 0.746 0.907 35
0.968 0.842 0.894 11



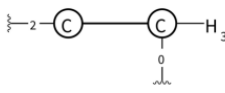
[CX4H2][CX4H2][CX3H0]
0.986 0.954 0.984 33
0.958 0.800 0.929 11



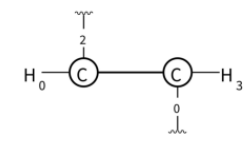
[#8][#6][#6][#8]
0.967 0.821 0.895 22
0.937 0.667 0.845 11



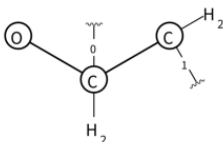
[#8][#6][#6]=[#8]
0.967 0.811 0.875 20
0.937 0.667 0.731 11



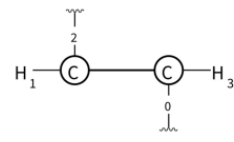
[CX4H3][CX3]
1.000 1.000 1.000 17
0.979 0.909 0.985 11



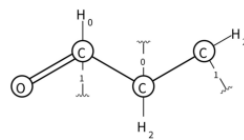
[CX4H3][CX3H0]
0.991 0.933 1.000 16
0.979 0.917 0.992 11



[CH2X4][O][CX4H2]
0.991 0.909 0.934 12
0.989 0.957 0.983 11



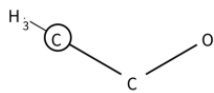
[CX4H3][CX4H1]
0.981 0.943 0.989 34
0.979 0.900 0.955 10



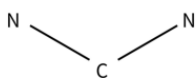
O=[CX3H0][CX4H2][CX4H2]
0.986 0.954 0.982 33
0.968 0.824 0.899 10



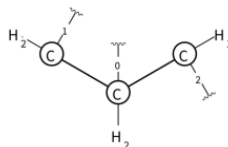
[#7H2][#6H0]
0.907 0.444 0.623 24
0.916 0.500 0.645 10



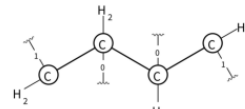
[CH3][#6][#8]
0.991 0.944 0.991 18
0.979 0.900 0.947 10



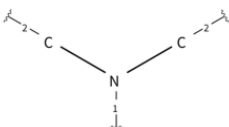
[#7][#6][#7]
0.963 0.667 0.960 16
0.947 0.667 0.891 10



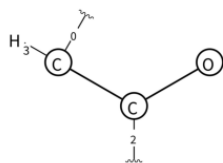
[CX4H2][CX4H2][CX4H1]
0.977 0.878 0.881 21
0.937 0.727 0.863 9



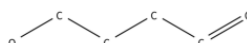
[CX4H2][CX4H2][CX4H2][CX4H2]
0.986 0.919 0.985 19
0.958 0.714 0.899 9



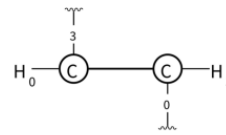
[#6X3][#7X3][#6X3]
0.925 0.429 0.499 18
0.916 0.600 0.610 9



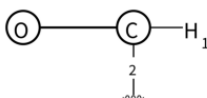
[CX4H3][CX4O]
0.991 0.941 0.990 17
0.979 0.889 0.988 9



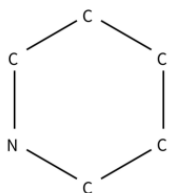
[#8][#6][#6][#6][#6]=[#8]
0.958 0.526 0.780 13
0.926 0.364 0.785 9



[CX4H3][CX4H0]
0.991 0.909 0.985 11
1.000 1.000 1.000 9



[CX4H]O
0.981 0.931 0.976 30
0.979 0.875 0.915 8



[#6]1[#6][#6][#6][#6]1
0.963 0.778 0.862 20
0.926 0.462 0.780 8



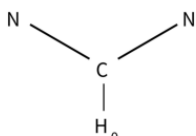
[#7H2][#6H2]
0.981 0.875 0.954 17
0.979 0.875 0.985 8



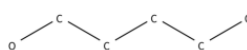
[#6H3][#7]
0.991 0.929 0.955 15
0.979 0.857 0.940 8



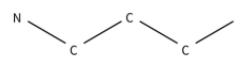
[#7X3][#6H3]
0.995 0.963 1.000 14
0.979 0.857 0.935 8



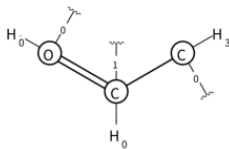
[#7][#6H0][#7]
0.967 0.696 0.905 14
0.947 0.545 0.864 8



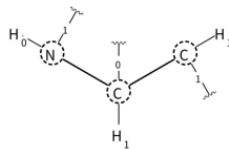
[#6][#6][#6][#6][#6][#8]
0.953 0.500 0.569 13
0.905 0.000 0.323 8



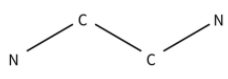
[#7][#6][#6][#6][#7]
0.967 0.533 0.735 11
0.937 0.500 0.686 8



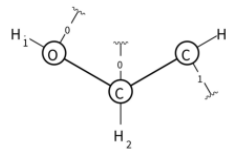
[OX1H0]=[CX3H0][CX4H3]
1.000 1.000 1.000 11
0.968 0.800 0.969 8



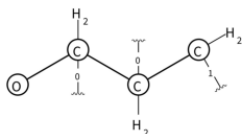
[CX3H1][#X2H0][CX3H1]
0.991 0.909 0.925 11
0.947 0.545 0.817 8



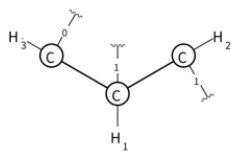
[#7][#6][#6][#7]
0.986 0.800 0.931 9
0.937 0.500 0.557 8



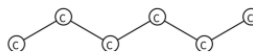
[CX4H2][OX2H1][CX4H2]
0.995 0.909 0.874 6
1.000 1.000 1.000 8



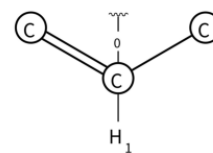
[CH2X4][O][CX4H2][CX4H2]
 1.000 1.000 1.000 5
 0.947 0.615 0.926 8



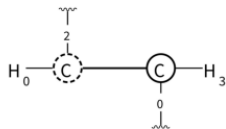
[CHX4][CH3X4][CH2X4]
 0.981 0.895 0.986 19
 0.968 0.769 0.844 7



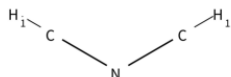
CCCCC
 0.967 0.800 0.843 19
 0.947 0.545 0.827 7



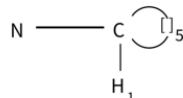
[CHX3](=C)C
 0.949 0.686 0.778 18
 0.968 0.727 0.755 7



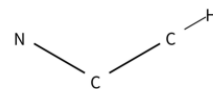
[CX4H3][CX3H0]
 1.000 1.000 1.000 15
 0.989 0.923 1.000 7



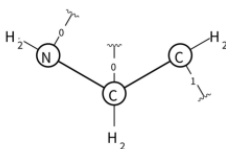
[#6H1][#7][#6H1]
 0.981 0.750 0.871 10
 0.926 0.364 0.681 7



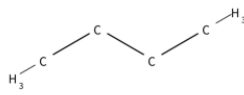
[#6H1r5][#7]
 0.972 0.571 0.896 10
 0.968 0.727 0.827 7



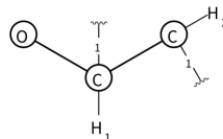
[#7][#6][#6H3]
 0.991 0.889 0.983 10
 0.958 0.600 0.916 7



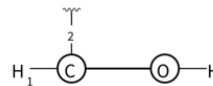
[CX4H2][NX3H2][CX4H2]
 0.991 0.889 0.988 9
 0.989 0.923 0.966 7



[#6H3][#6][#6][#6H3]
 0.981 0.714 0.785 8
 0.958 0.600 0.721 7



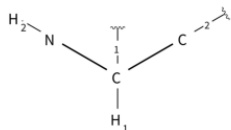
O[CX4H][CX4H2]
 0.986 0.927 0.975 22
 0.979 0.833 0.955 6



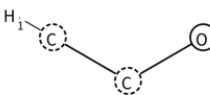
[OH][CX4H]
 0.972 0.864 0.857 21
 0.958 0.500 0.675 6



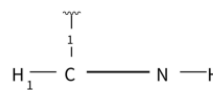
[#7H2][#6H1]
 0.958 0.727 0.949 19
 0.968 0.727 0.925 6



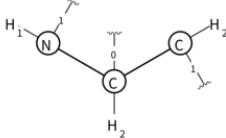
[#7H2][#6X4H1][#6X3]
 0.981 0.875 0.984 18
 0.979 0.800 0.899 6



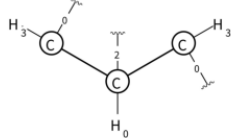
[CH]cO
 0.972 0.786 0.948 17
 0.937 0.625 0.745 6



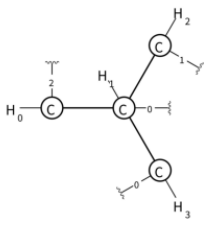
[#7H][#6X3H1]
 0.944 0.143 0.476 11
 0.926 0.000 0.362 6



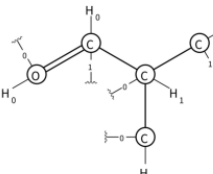
[CX4H2][NX3H1][CX4H2]
 0.986 0.800 0.856 9
 0.968 0.667 0.862 6



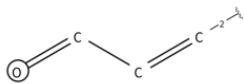
[CX4H3][CX4H0][CX4H3]
 1.000 1.000 1.000 7
 0.979 0.800 0.913 6



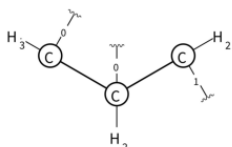
[CX4H1][CX4H3][CX4H2][CX3H0]
 1.000 0 0
 0.937 0.000 0.858 6



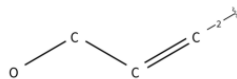
[OX1H0]=[CX3H0][CX4H1][CX4H3][CX4H2]
 1.000 0 0
 0.937 0.000 0.887 6



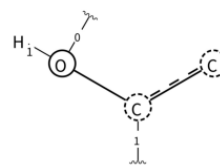
O=[#6][#6]=[#6X3]
0.972 0.824 0.952 17
0.989 0.889 0.938 5



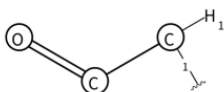
[CX4H2][CX4H3][CX4H2]
0.991 0.938 0.993 16
0.989 0.909 0.963 5



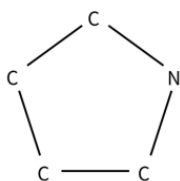
[#8][#6][#6]=[#6X3]
0.981 0.867 0.937 16
0.979 0.750 0.805 5



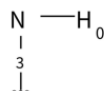
[OX2H][cX3]:[c]
0.963 0.636 0.958 15
0.947 0.615 0.614 5



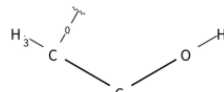
O=C[CX3H]
0.972 0.700 0.907 12
0.979 0.750 1.000 5



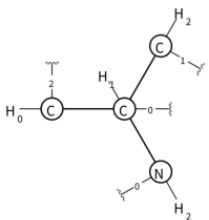
[#6]1[#6][#6][#6][#7]1
0.963 0.500 0.752 11
0.947 0.444 0.675 5



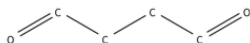
[#7X3H0]
0.981 0.800 0.868 11
0.968 0.667 0.558 5



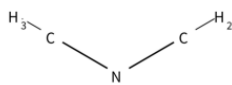
[#6X4H3][#6][#8H]
0.986 0.842 0.980 10
0.989 0.909 1.000 5



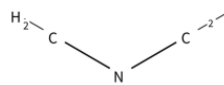
[CX4H1][NX3H2][CX4H2][CX3H0]
0.977 0.667 0.938 10
0.979 0.750 0.894 5



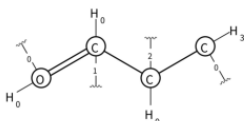
[#8]=[#6][#6][#6][#6]=[#8]
0.977 0.667 0.774 10
0.947 0.000 0.813 5



[#6H3][#7][#6H2]
0.986 0.769 0.959 7
0.968 0.571 1.000 5



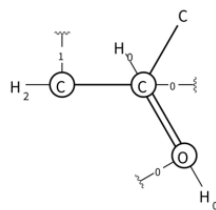
[#6H2][#7][#6X3]
0.991 0.857 0.785 7
0.979 0.750 0.861 5



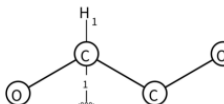
[OX1H0]=[CX3H0][CX4H0][CX4H3]
1.000 1.000 1.000 4
0.968 0.571 1.000 5



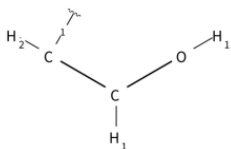
[#7][#6][#6][#6][#6][#7]
0.986 0.400 0.615 4
0.937 0.000 0.425 5



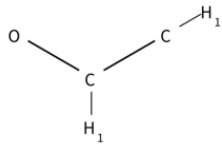
[OX1H0]=[CX3H0][#6][CX4H2]
1.000 1.000 1.000 18
0.979 0.750 0.944 4



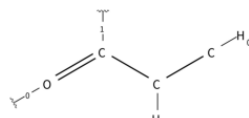
[CX4H](O)CO
0.972 0.769 0.881 14
0.979 0.667 0.852 4



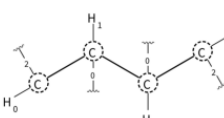
[#6X4H2][#6H1][#8H]
0.986 0.897 0.969 14
0.968 0.400 0.835 4



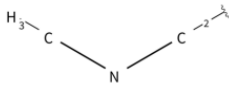
[#8][#6H1][#6H1]
0.944 0.333 0.592 14
0.989 0.889 1.000 4



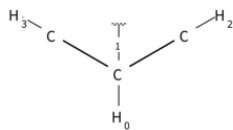
[#8X1]=[#6X3][#6H2][#6H0]
0.986 0.800 0.875 9
0.989 0.857 0.944 4



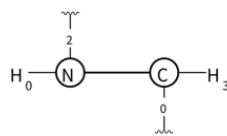
[cX3H0][cX3H1][cX3H1][cX3H0]
0.977 0.615 0.864 9
0.968 0.400 0.449 4



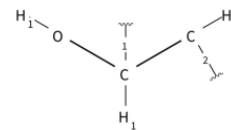
[#6H3][#7][#6X3]
 0.995 0.941 1.000 9
 0.968 0.571 0.747 4



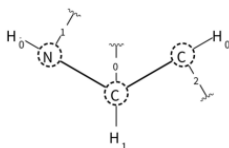
[#6H3][#6X3H0][#6H2]
 1.000 1.000 1.000 8
 0.979 0.667 1.000 4



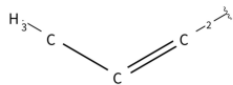
[CX4H3][NX3H0]
 0.981 0.714 0.949 8
 0.979 0.667 0.729 4



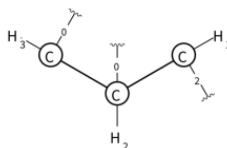
[#8H][#6X4H1][#6X3H0]
 0.986 0.769 0.938 8
 0.979 0.667 0.842 4



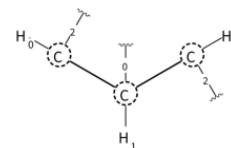
[cX3H1][nx2H0][cX3H0]
 0.986 0.769 0.885 7
 0.968 0.400 0.731 4



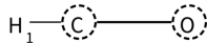
[#6H3][#6]=[#6X3]
 1.000 1.000 1.000 6
 1.000 1.000 1.000 4



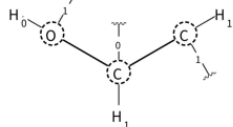
[CX4H2][CX4H3][CX4H1]
 0.991 0.833 0.858 6
 0.979 0.750 0.811 4



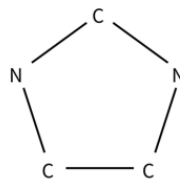
[cX3H1][cX3H0][cX3H0]
 0.972 0.000 0.382 6
 0.958 0.000 0.578 4



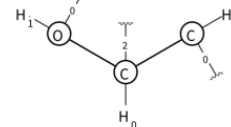
c[CH]
 0.977 0.000 0.798 5
 0.968 0.400 0.767 4



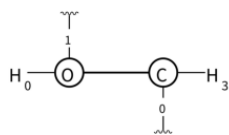
[cX3H1][ox2H0][cX3H1]
 0.991 0.750 0.812 5
 1.000 1.000 1.000 4



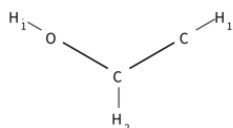
[#6]1[#6][#7][#6][#7]1
 0.991 0.000 0.871 4
 0.968 0.400 0.641 4



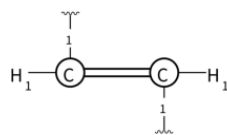
[OX2H1][CX4H0][CX4H3]
 1.000 1.000 1.000 2
 1.000 1.000 1.000 4



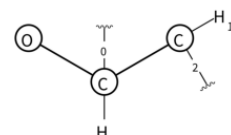
[CX4H3][OX2H0]
 0.991 0.952 0.990 20
 0.979 0.500 0.711 3



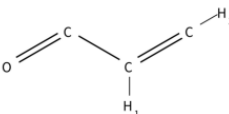
[#8H][#6H2][#6H1]
 0.986 0.870 0.955 12
 0.979 0.500 1.000 3



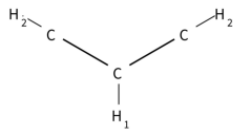
[CHX3]=[CHX3]
 0.972 0.700 0.766 12
 0.989 0.800 0.699 3



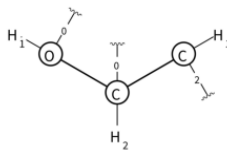
[CX4H2](O)[CHX4]
 0.977 0.706 0.927 11
 0.989 0.800 0.850 3



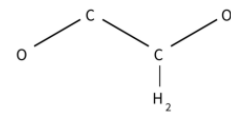
[#8]=[#6][#6H1]=[#6H1]
 0.972 0.625 0.824 10
 0.979 0.500 0.903 3



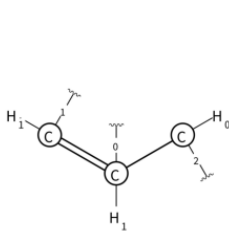
[#6H1][#6H2][#6H2]
 0.972 0.571 0.812 10
 0.979 0.500 0.492 3



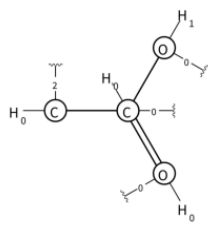
[CX4H2][OX2H1][CX4H1]
 0.991 0.889 0.957 10
 0.979 0.667 0.514 3



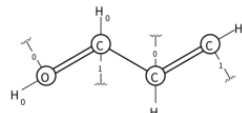
[#8][#6][#6H2][#8]
 0.991 0.875 0.959 9
 1.000 1.000 1.000 3



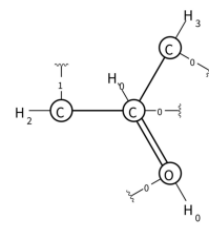
[CX3H1](=[CX3H1])[CX3H0]
0.977 0.615 0.662 9
0.979 0.500 0.589 3



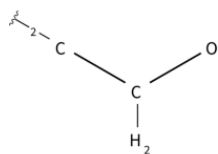
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]
0.986 0.842 0.899 9
1.000 1.000 1.000 3



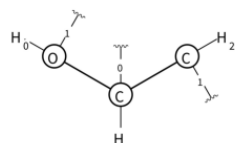
[OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.981 0.714 0.849 9
0.979 0.500 0.733 3



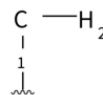
[CX3H0](=[OX1H0])([CX4H3])[CX4H2]
1.000 1.000 1.000 8
0.989 0.800 1.000 3



[#6X3][#6H2][#8]
0.995 0.933 1.000 8
1.000 1.000 1.000 3



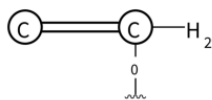
[CX4H2]([OX2H0])[CX4H2]
0.995 0.923 1.000 7
0.989 0.857 1.000 3



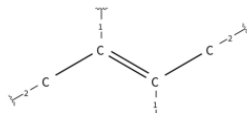
[#6X3H2]
0.995 0.909 1.000 6
0.979 0.667 0.903 3



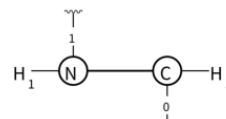
[cX3H1]([nX3H1])[cX3H1]
0.977 0.286 0.441 6
0.968 0.000 0.200 3



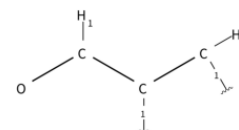
[CH2X3](=C)
0.995 0.909 1.000 6
0.979 0.667 0.711 3



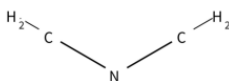
[#6X3][#6X3]=[#6X3][#6X3]
0.977 0.286 0.522 6
0.968 0.000 0.168 3



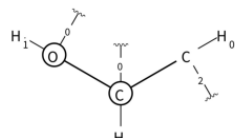
[CX4H3][NX3H1]
0.991 0.750 0.827 5
0.968 0.000 0.903 3



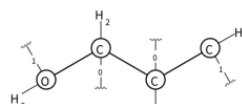
[#8][#6H][#6X3][#6X3H]
0.977 0.000 0.781 5
0.968 0.000 0.764 3



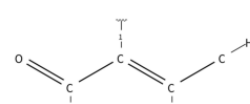
[#6H2][#7][#6H2]
0.986 0.667 0.798 5
0.968 0.000 0.764 3



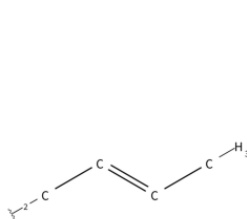
[OX2H1][CX4H2][#6X3H0]
0.991 0.667 0.852 4
0.989 0.800 1.000 3



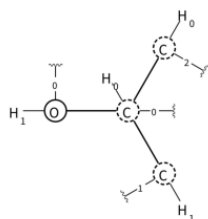
[OX2H0][CX4H2][CX4H2][CX4H2]
1.000 1.000 1.000 4
0.989 0.800 1.000 3



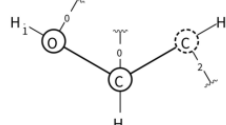
[#8]=[#6X3][#6X3]=[#6X3][#6H3]
1.000 1.000 1.000 4
1.000 1.000 1.000 3



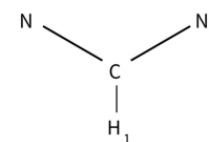
[#6X3][#6]=[#6][#6H3]
0.995 0.889 0.944 4
0.979 0.500 1.000 3



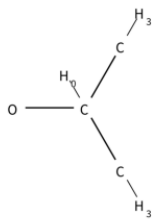
[cX3H0]([cX3H1])([cX3H0])([OX2H1]
0.981 0.000 0.707 4
0.979 0.500 0.519 3



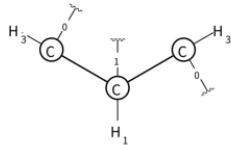
[CX4H2]([OX2H1])[cX3H0]
0.995 0.800 1.000 3
1.000 1.000 1.000 3



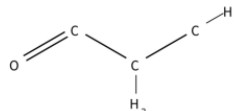
[#7][#6H1][#7]
0.995 0.667 1.000 2
0.979 0.500 0.850 3



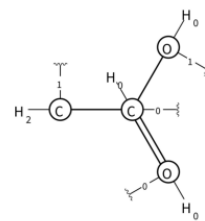
[#6H0][[#6H3]][[#6H3]][#8]
1.000 1.000 1.000 2
0.989 0.800 0.903 3



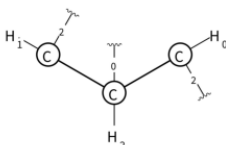
[CHX4][[CH3X4]][CH3X4]
0.995 0.966 0.992 15
0.979 0.500 0.708 2



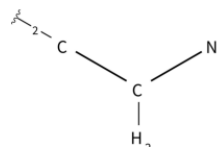
[#8]=[#6][#6H2][#6H1]
0.963 0.333 0.960 10
0.989 0.667 1.000 2



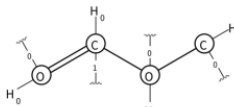
[CX3H0]=[OX1H0][OX2H0][CX4H2]
0.995 0.933 0.944 8
0.989 0.800 1.000 2



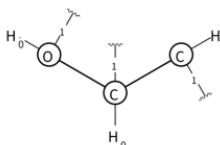
[CX4H2][[CX4H1]][CX3H0]
0.981 0.667 0.897 8
0.989 0.667 1.000 2



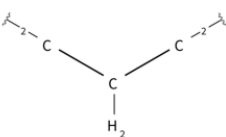
[#6X3][#6H2][#7]
0.991 0.857 1.000 8
0.979 0.000 1.000 2



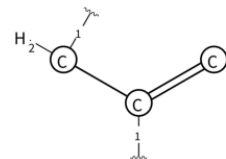
[OX1H0]=[CX3H0][OX2H0][CX4H3]
1.000 1.000 1.000 8
0.968 0.000 0.140 2



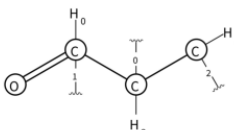
[OX2H0][CX3H0][CX4H2]
0.991 0.857 0.985 8
0.958 0.333 0.662 2



[#6X3][#6H2][#6X3]
0.995 0.933 0.985 8
0.979 0.500 0.184 2



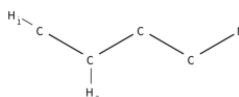
[CX4H2][CX3]=C
1.000 1.000 1.000 8
0.989 0.800 1.000 2



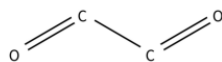
O=[CX3H0][CX4H2][CX4H1]
0.977 0.545 0.969 8
0.989 0.667 1.000 2



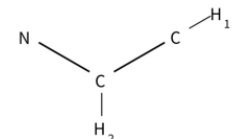
O=[CX3]
0.977 0.444 0.750 7
0.968 0.000 0.223 2



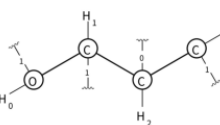
[#6H1][#6H2][#6][#6][#7]
0.986 0.667 0.974 6
0.968 0.400 0.708 2



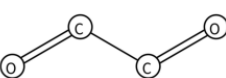
[#8]=[#6][#6][#8]
0.991 0.800 0.863 6
1.000 1.000 1.000 2



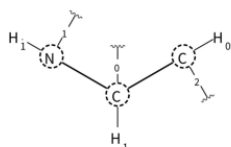
[#7][#6H2][#6H1]
0.977 0.444 0.669 6
1.000 1.000 1.000 2



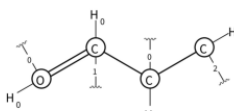
[OX2H0][CX4H1][CX4H2][CX4H2]
0.986 0.667 1.000 6
0.989 0.667 1.000 2



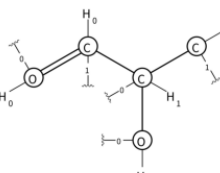
O=CC=O
0.995 0.909 0.878 6
1.000 1.000 1.000 2



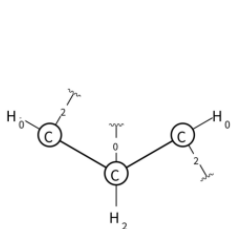
[CX3H1][[nX3H1]][CX3H0]
0.977 0.000 0.657 5
0.979 0.000 0.109 2



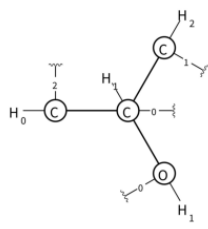
[OX1H0]=[CX3H0][CX4H2][CX3H0]
1.000 1.000 1.000 5
0.989 0.667 0.633 2



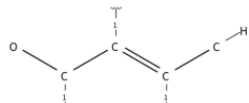
[OX1H0]=[CX3H0][CX4H1][OX2H1][CX4H2]
0.995 0.889 0.963 5
0.989 0.667 1.000 2



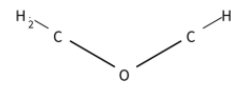
[CX4H2][CX3H0][CX3H0]
1.000 1.000 1.000 5
0.989 0.667 0.792 2



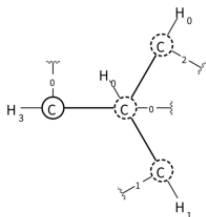
[CX4H1][OX2H1][CX4H2][CX3H0]
0.991 0.750 0.878 5
1.000 1.000 1.000 2



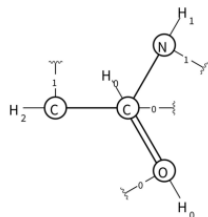
[#8][#6X3][#6X3]=[#6X3][#6H3]
1.000 1.000 1.000 4
1.000 1.000 1.000 2



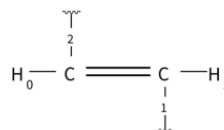
[#6H2][#8][#6H1]
1.000 1.000 1.000 4
0.989 0.667 1.000 2



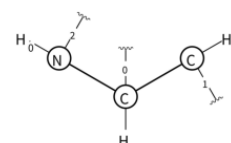
[cX3H0][cX3H1][cX3H0][CX4H3]
0.986 0.571 0.811 4
0.989 0.667 1.000 2



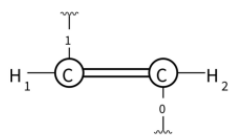
[CX3H0]=[OX1H0][NX3H1][CX4H2]
0.981 0.000 0.527 4
0.979 0.000 0.578 2



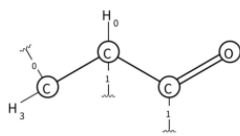
[#6X3H1]=[#6X3H0]
1.000 1.000 1.000 4
0.989 0.667 0.613 2



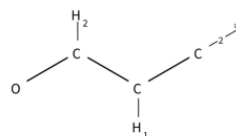
[CX4H2][NX3H0][CX4H2]
0.995 0.800 1.000 3
0.979 0.000 0.792 2



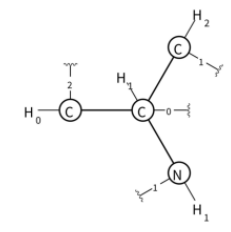
[CX3H2]=[CX3H1]
1.000 1.000 1.000 3
1.000 1.000 1.000 2



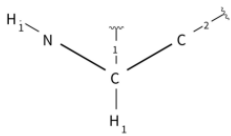
[CX4H3][CX3H0][CX3]=O
1.000 1.000 1.000 3
1.000 1.000 1.000 2



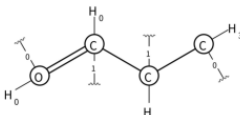
[#8][#6H2][#6H][#6X3]
0.995 0.800 1.000 3
0.979 0.000 1.000 2



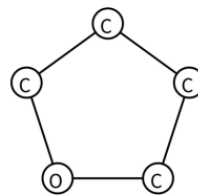
[CX4H1][NX3H1][CX4H2][CX3H0]
0.991 0.500 1.000 3
0.979 0.000 0.333 2



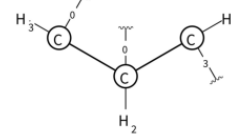
[#7H1][#6X4H1][#6X3]
0.986 0.000 0.903 3
0.979 0.000 0.417 2



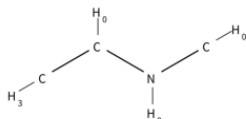
[OX1H0]=[CX3H0][CX3H0][CX4H3]
0.995 0.800 1.000 3
1.000 1.000 1.000 2



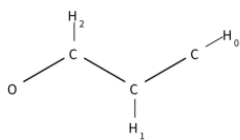
C1OCCCC1
0.991 0.500 1.000 3
0.989 0.667 1.000 2



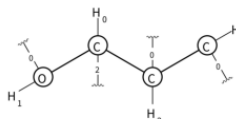
[CX4H2][CX4H3][CX4H0]
1.000 1.000 1.000 2
0.989 0.800 0.792 2



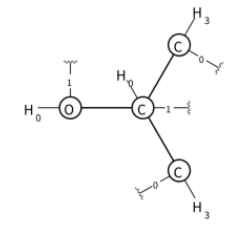
[#6H3][#6H0][#7H0][#6H0]
0.995 0.667 1.000 2
0.979 0.000 0.292 2



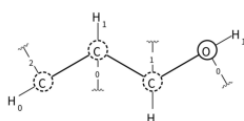
[#8][#6H2][#6H1][#6H0]
1.000 1.000 1.000 2
0.979 0.000 0.792 2



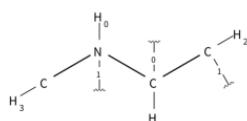
[OX2H1][CX4H0][CX4H2][CX4H3]
1.000 1.000 1.000 2
0.989 0.800 0.417 2



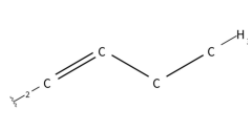
[CX4H3][CX4H0][CX4H3][OX2H0]
1.000 1.000 1.000 2
0.989 0.667 0.662 2



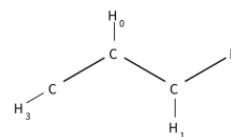
[CX3H0][CX3H1][CX3H0][OX2H1]
 0.995 0.667 0.662 2
 0.979 0.000 0.333 2



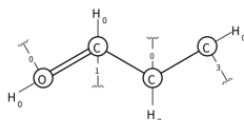
[#6H3][#7X3H0][#6X4H2][#6X4H2]
 1.000 1.000 1.000 2
 0.979 0.000 1.000 2



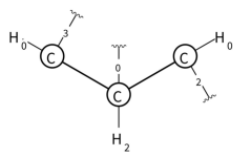
[#6X3]=[#6][#6][#6H3]
 1.000 1.000 1.000 2
 1.000 1.000 1.000 2



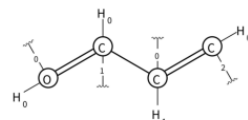
[#6H3][#6H0][#6H1][#7]
 0.995 0.667 1.000 2
 0.968 0.000 0.217 2



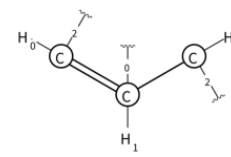
[OX1H0]=[CX3H0][CX4H2][CX4H0]
 0.995 0.000 0.100 1
 1.000 1.000 1.000 2



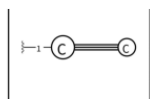
[CX4H2][CX4H0][CX3H0]
 0.995 0.000 1.000 1
 1.000 1.000 1.000 2



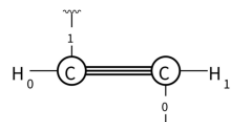
[OX1H0]=[CX3H0][CX3H1]=[CX3H0]
 1.000 1.000 1.000 1
 0.979 0.000 1.000 2



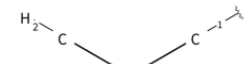
[CX3H1]=[CX3H0][CX3H0]
 1.000 1.000 1.000 1
 0.979 0.000 1.000 2



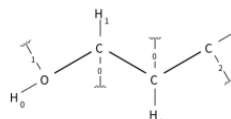
[\$([CX2]#C)]
 1.000 1.000 1.000 1
 1.000 1.000 1.000 2



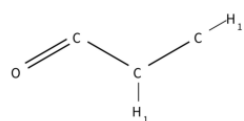
[CX2H1]#CX2H0
 1.000 - 0 0
 0.989 0.667 1.000 2



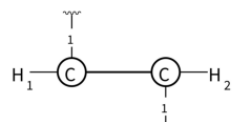
[#6H2][#6][#6X2]
 1.000 1.000 1.000 0
 0.979 0.000 1.000 2



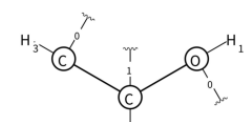
[#8X2H0][#6X3H1][#6X3H1][#6X3H0]
 1.000 - 0 0
 0.979 0.000 0.633 2



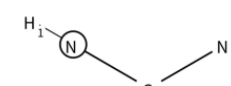
[#8]=[#6][#6H1][#6H1]
 0.967 0.632 0.659 12
 0.958 0.000 0.029 1



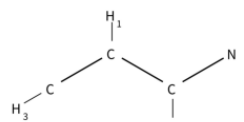
[CX4H2][CX3H]
 0.977 0.667 0.784 10
 1.000 1.000 1.000 1



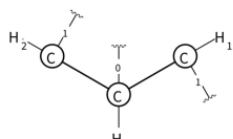
[CX4H3][CX4H1][OX2H1]
 0.995 0.933 1.000 8
 1.000 1.000 1.000 1



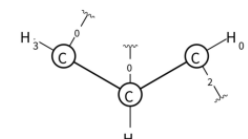
[NH1][#6][#7]
 0.986 0.727 1.000 7
 0.989 0.000 1.000 1



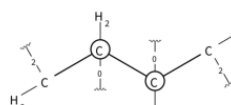
[#6H3][#6H1][#6H1][#7]
 0.972 0.250 0.617 7
 0.989 0.000 1.000 1



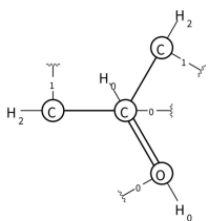
[CX4H2][CX4H2][CX3H1]
 0.986 0.667 0.754 6
 1.000 1.000 1.000 1



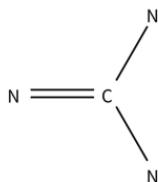
[CX4H2][CX4H3][CX3H0]
 1.000 1.000 1.000 5
 1.000 1.000 1.000 1



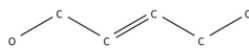
[#6X3H0][CX4H2][CX4H2][#6X3H0]
 0.995 0.889 1.000 5
 0.989 0.000 0.250 1



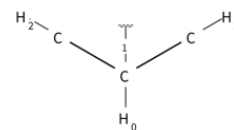
[CX3H0]=[OX1H0][CX4H2][CX4H2]
 1.000 1.000 1.000 5
 1.000 1.000 1.000 1



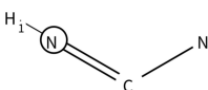
[#7][#6][#7]=[#7]
 0.991 0.750 1.000 5
 0.989 0.000 0.083 1



[#8][#6][#6]=[#6][#6][#8]
 0.977 0.000 0.938 5
 0.989 0.000 0.083 1



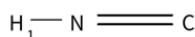
[#6H2][#6X3H0][#6H2]
 1.000 1.000 1.000 5
 1.000 1.000 1.000 1



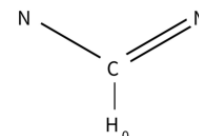
[NH1]=[#6][#7]
 1.000 1.000 1.000 5
 0.979 0.000 0.100 1



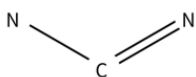
[#8]=[#6][#6]=[#6][#6]=[#8]
 0.986 0.571 0.918 5
 0.989 0.000 1.000 1



[#6]=[#7H]
 0.995 0.889 1.000 5
 0.979 0.000 0.083 1



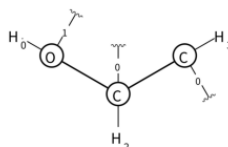
[#7][#6H0]=[#7]
 1.000 1.000 1.000 5
 0.979 0.000 0.083 1



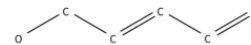
[#7][#6]=[#7]
 1.000 1.000 1.000 5
 0.979 0.000 0.071 1



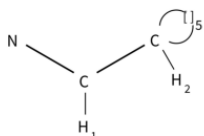
[#6][#7]
 1.000 1.000 1.000 4
 1.000 1.000 1.000 1



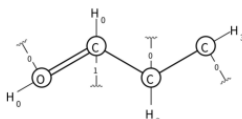
[CX4H2][OX2H0][CX4H3]
 1.000 1.000 1.000 4
 1.000 1.000 1.000 1



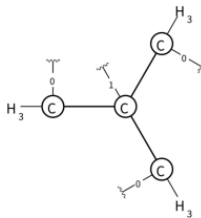
[#8][#6][#6]=[#6][#6]=[#8]
 0.981 0.000 0.811 4
 0.989 0.000 1.000 1



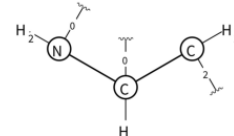
[#7][#6H1][#6H2r5]
 0.995 0.857 1.000 4
 0.989 0.667 0.250 1



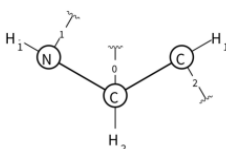
[OX1H0]=[CX3H0][CX4H2][CX4H3]
 1.000 1.000 1.000 4
 1.000 1.000 1.000 1



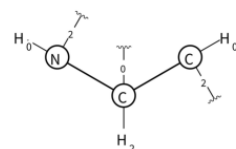
[CX4H2][CX4H3][CX4H3][CX4H3]
 1.000 1.000 1.000 4
 0.989 0.667 0.250 1



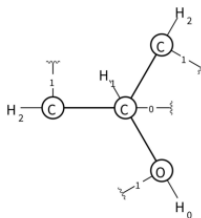
[CX4H2][NX3H2][CX4H1]
 0.995 0.800 0.817 3
 0.989 0.000 1.000 1



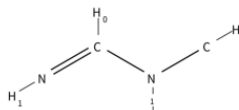
[CX4H2][NX3H1][CX4H1]
 0.986 0.000 0.314 3
 0.989 0.000 0.071 1



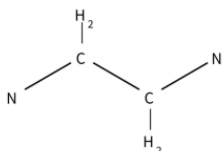
[CX4H2][NX3H0][CX3H0]
 1.000 1.000 1.000 3
 0.989 0.000 1.000 1



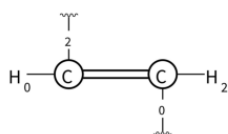
[CX4H1][OX2H0][CX4H2][CX4H2]
 1.000 1.000 1.000 3
 0.989 0.000 1.000 1



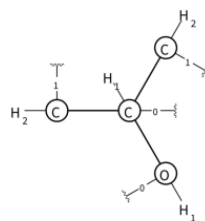
[#7H1]=[#6H0][#7X3][#6H3]
 1.000 1.000 1.000 3
 0.989 0.000 1.000 1



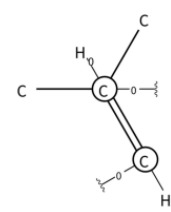
[#7][#6H2][#6H2][#7]
 1.000 1.000 1.000 3
 0.979 0.000 0.100 1



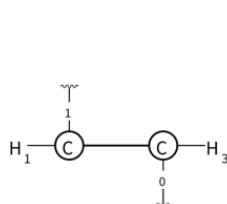
[CX3H2]=[CX3H0]
 0.995 0.800 1.000 3
 0.979 0.000 0.167 1



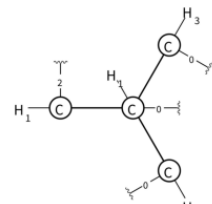
[CX4H1]([OX2H1])([CX4H2])[CX4H2]
 0.991 0.500 1.000 3
 0.989 0.000 1.000 1



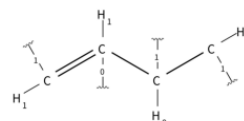
[CX3H2]=[CX3H0]([#6])([#6])
 0.995 0.800 1.000 3
 0.989 0.000 1.000 1



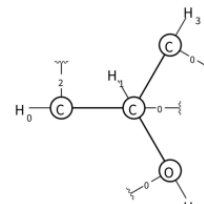
[CX4H3][CX3H1]
 1.000 1.000 1.000 3
 1.000 1.000 1.000 1



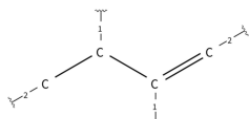
[CX4H1]([CX4H3])([CX4H3])[CX4H1]
 1.000 1.000 1.000 2
 0.989 0.000 1.000 1



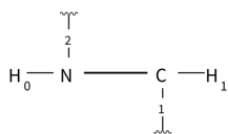
[#6X3H1]=[#6X3H1][#6X3H0][#6X3H1]
 0.991 0.000 0.333 2
 0.989 0.000 0.036 1



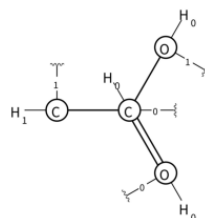
[CX4H1]([OX2H1])([CX4H3])[CX3H0]
 1.000 1.000 1.000 2
 1.000 1.000 1.000 1



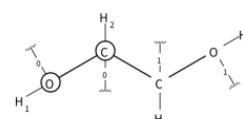
[#6X3][#6X3][#6X3]=[#6X3]
 0.995 0.667 0.662 2
 0.989 0.000 0.045 1



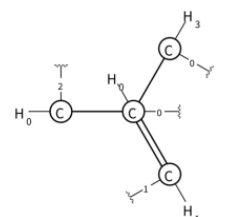
[#6X3H1][#7X3H0]
 0.995 0.667 1.000 2
 1.000 1.000 1.000 1



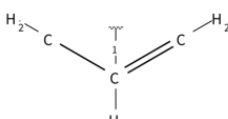
[CX3H0](=[OX1H0])([OX2H0])[CX3H1]
 0.995 0.667 1.000 2
 0.989 0.000 0.250 1



[OX2H1][CX4H2][#6X3H0][#8X2H0]
 0.995 0.667 1.000 2
 1.000 1.000 1.000 1



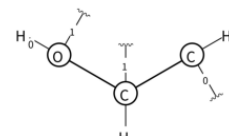
[CX3H0](=[CX3H1])([CX4H3])[CX3H0]
 1.000 1.000 1.000 2
 0.979 0.000 0.250 1



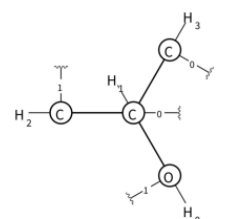
[#6H2][#6X3H0]=[#6H2]
 1.000 1.000 1.000 2
 0.989 0.000 1.000 1



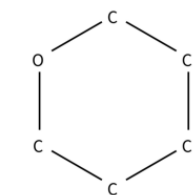
[#6H2][#6X2]
 0.995 0.667 1.000 2
 1.000 1.000 1.000 1



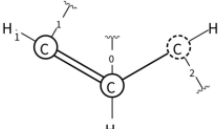
[OX2H0][CX4H1][CX4H3]
 1.000 1.000 1.000 2
 1.000 1.000 1.000 1



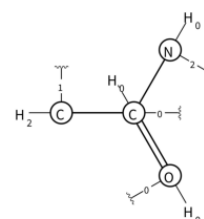
[CX4H1]([OX2H0])([CX4H3])[CX4H2]
 1.000 1.000 1.000 2
 1.000 1.000 1.000 1



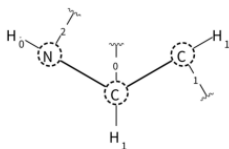
[#8]1[#6][#6][#6][#6][#6]1
 0.995 0.667 1.000 2
 0.979 0.000 0.050 1



[CX3H1](=[CX3H1])[CX3H0]
 0.995 0.000 1.000 1
 0.989 0.000 0.045 1



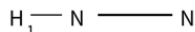
[CX3H0](=[OX1H0])([NX3H0])[CX4H2]
 0.995 0.000 0.125 1
 0.989 0.000 0.100 1



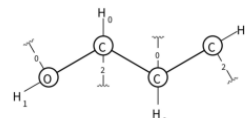
[cX3H1]([nX3H0])[cX3H1]
 0.995 0.000 0.167 1
 1.000 1.000 1.000 1



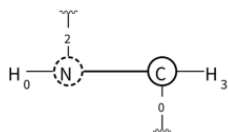
[#7][#7]
 0.995 0.000 0.062 1
 0.979 0.000 0.125 1



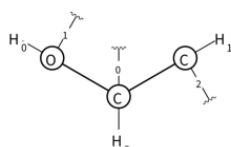
[#7][#7H1]
 0.995 0.000 0.071 1
 0.989 0.000 0.056 1



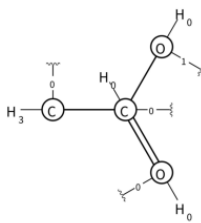
[OX2H1][CX4H0][CX4H2][CX3H0]
 0.995 0.000 0.125 1
 0.989 0.000 1.000 1



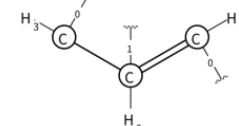
[CX4H3][nX3H0]
 1.000 1.000 1.000 1
 1.000 1.000 1.000 1



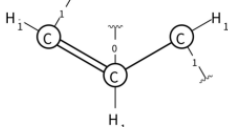
[CX4H2]([OX2H0])[CX4H1]
 1.000 1.000 1.000 1
 0.989 0.000 1.000 1



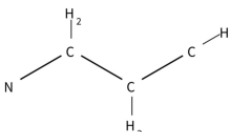
[CX3H0](=[OX1H0])([OX2H0])[CX4H3]
 1.000 1.000 1.000 1
 0.989 0.000 0.125 1



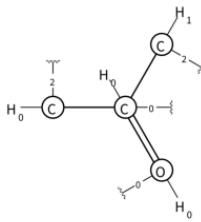
[CX4H3][CX3H0]=[CX3H2]
 0.995 0.000 1.000 1
 0.979 0.500 0.167 1



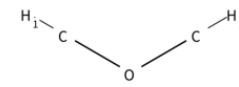
[CX3H1](=[CX3H1])[CX3H1]
 0.995 0.000 0.125 1
 0.989 0.000 0.250 1



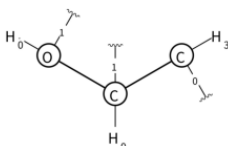
[#7][#6H2][#6H2][#6H1]
 0.995 0.000 1.000 1
 1.000 1.000 1.000 1



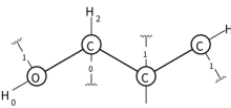
[CX3H0](=[OX1H0])([CX4H1])[CX3H0]
 1.000 1.000 1.000 1
 1.000 1.000 1.000 1



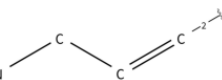
[#6H][#8][#6H]
 1.000 1.000 1.000 1
 1.000 1.000 1.000 1



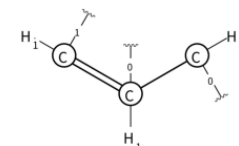
[OX2H0][CX3H0][CX4H3]
 1.000 1.000 1.000 1
 0.989 0.000 0.250 1



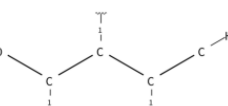
[OX2H0][CX4H2][CX4H1][CX4H2]
 1.000 1.000 1.000 1
 0.989 0.000 0.250 1



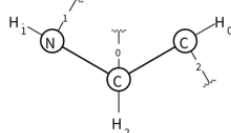
[#7][#6][#6]=[#6X3]
 1.000 1.000 1.000 1
 0.989 0.000 0.056 1



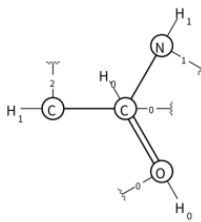
[CX3H1](=[CX3H1])[CX4H3]
 0.995 0.667 1.000 1
 0.989 0.000 1.000 1



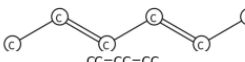
[#8][#6X3][#6X3][#6X3][#6H3]
 1.000 1.000 1.000 1
 0.989 0.000 1.000 1



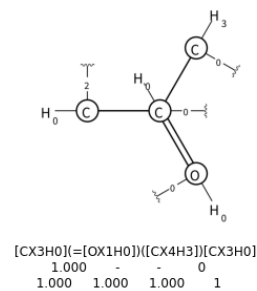
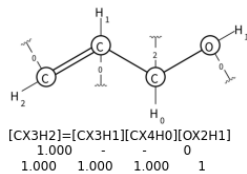
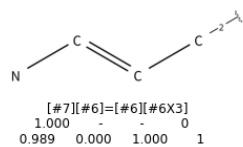
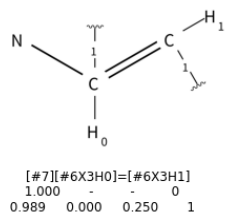
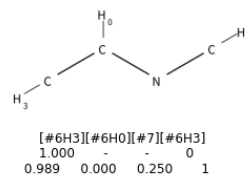
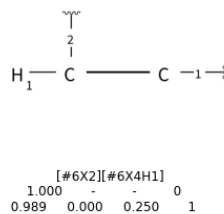
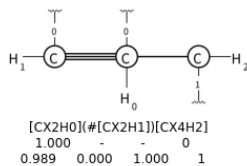
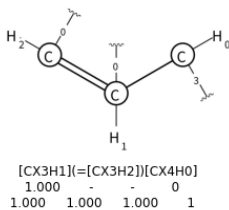
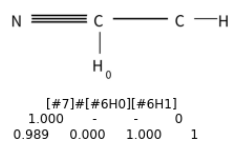
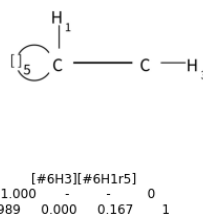
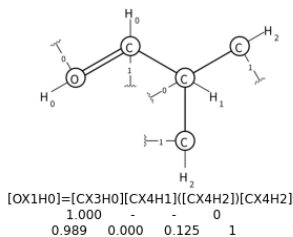
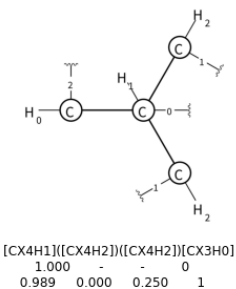
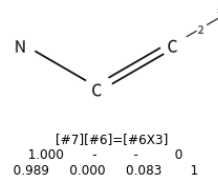
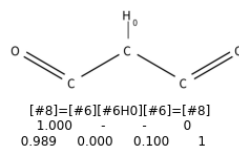
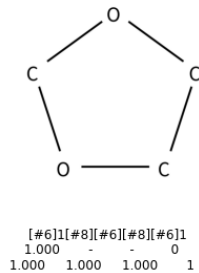
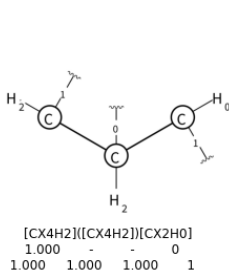
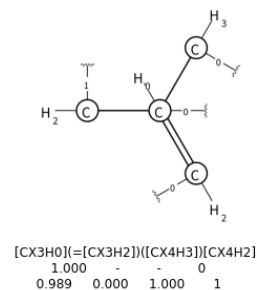
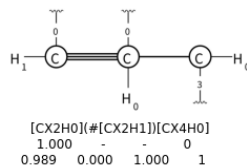
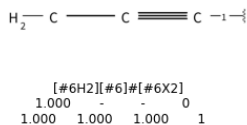
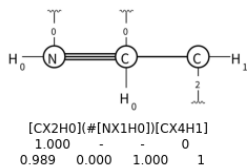
[CX4H2]([NX3H1])[CX3H0]
 1.000 1.000 1.000 1
 0.989 0.000 1.000 1

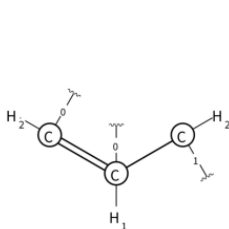


[CX3H0](=[OX1H0])([NX3H1])[CX4H1]
 1.000 0.000 1.000 0
 0.989 0.000 1.000 1

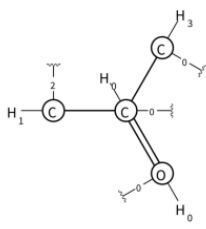


CC=CC=CC
 1.000 0.000 0.100 0
 0.989 0.000 1.000 1

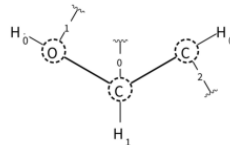




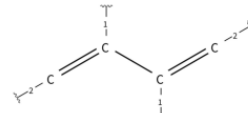
[CX3H1]=[CX3H2]][CX4H2]
 1.000 - - 0
 0.989 0.000 1.000 1



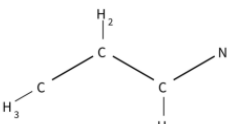
[CX3H0]=[OX1H0]][CX4H3]][CX4H1]
 1.000 - - 0
 0.989 0.000 1.000 1



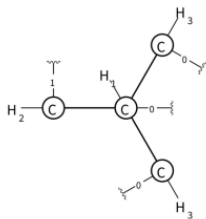
[cX3H1][[oX2H0]][cX3H0]
 1.000 - - 0
 0.989 0.000 1.000 1



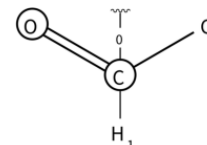
[#6X3]=[#6X3][#6X3]=[#6X3]
 1.000 - - 0
 0.989 0.000 0.125 1



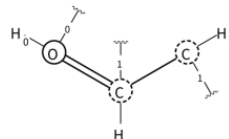
[#6H3][#6H2][#6H1][#7]
 1.000 - - 0
 0.989 0.000 1.000 1



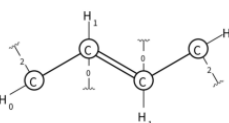
[CX4H1]][CX4H3]][CX4H3]][CX4H2]
 0.995 0.941 0.988 9
 1.000 - - 0



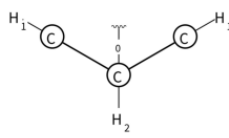
[CX3H1]=[O][#6]
 1.000 1.000 1.000 8
 1.000 - - 0



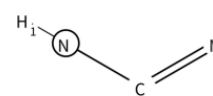
[OX1H0]=[cX3H0]][cX3H1]
 0.977 0.286 0.639 5
 0.989 - - 0



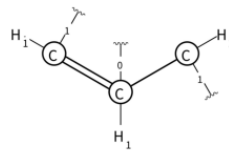
[CX3H0]][CX3H1]=[CX3H1]][CX3H0]
 0.981 0.333 0.693 5
 1.000 - - 0



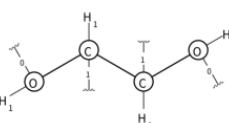
[CX4H2]][[CH]][[CH]
 0.991 0.750 0.865 5
 0.989 - - 0



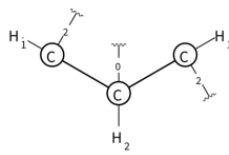
[NH1][[#6]=[#7]
 1.000 1.000 1.000 5
 1.000 - - 0



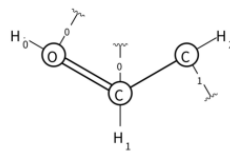
[CX3H1]=[CX3H1]][CX4H2]
 1.000 1.000 1.000 5
 1.000 - - 0



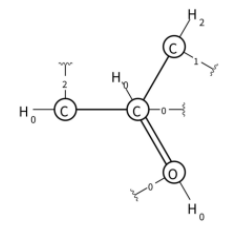
[OX2H1]][CX4H1]][CX4H1]][OX2H1]
 1.000 1.000 1.000 5
 1.000 - - 0



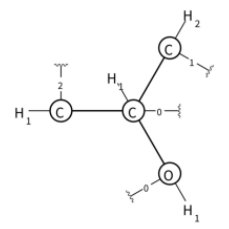
[CX4H2]][[CX4H1]][[CX4H1]
 0.995 0.857 1.000 4
 0.989 - - 0



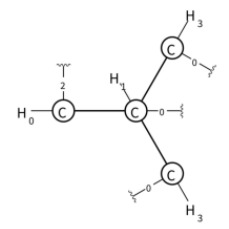
[CX3H1]=[OX1H0]][CX4H2]
 0.986 0.400 0.820 4
 1.000 - - 0



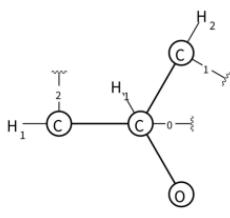
[CX3H0]=[OX1H0]][[CX4H2]][CX3H0]
 1.000 1.000 1.000 4
 0.989 - - 0



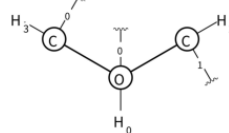
[CX4H1]][[OX2H1]][[CX4H2]][CX4H1]
 0.991 0.667 0.871 4
 1.000 - - 0



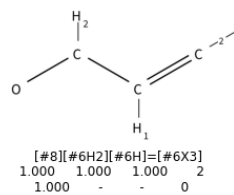
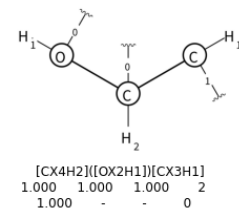
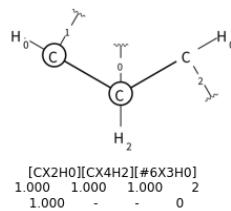
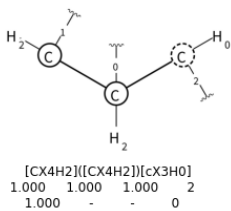
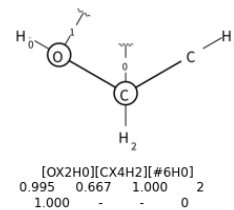
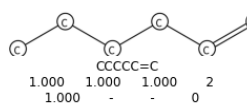
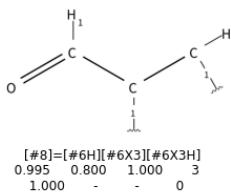
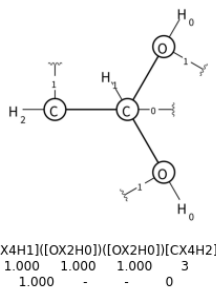
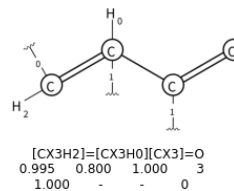
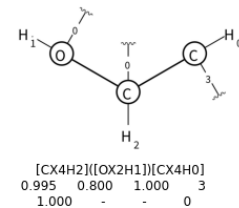
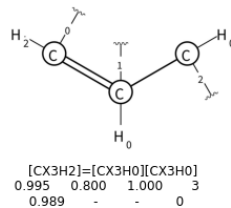
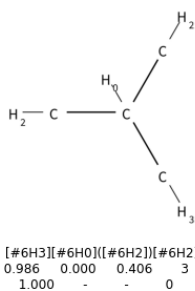
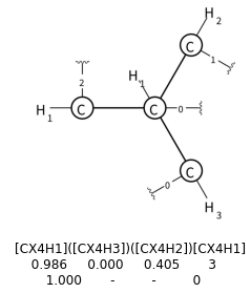
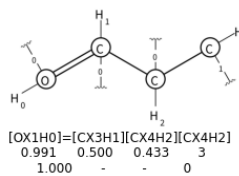
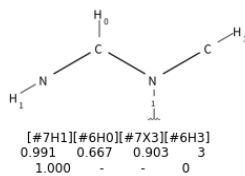
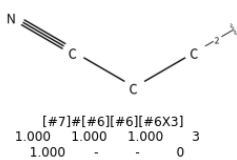
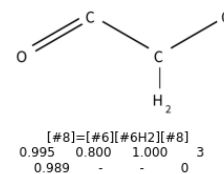
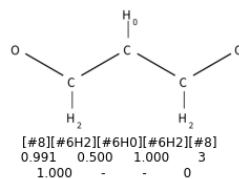
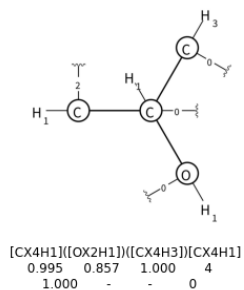
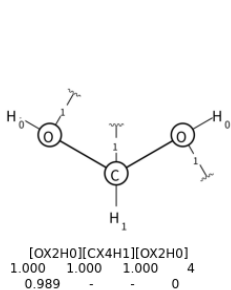
[CX4H1]][[CX4H3]][[CX4H3]][CX3H0]
 0.995 0.857 1.000 4
 0.989 - - 0

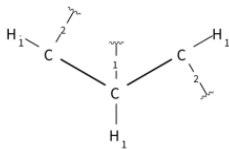


O[CX4H]][[CX4H2]][CX4H1]
 0.991 0.667 0.871 4
 0.989 - - 0

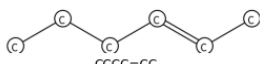


[CX4H3][OX2H0]][CX4H2]
 0.995 0.857 0.944 4
 1.000 - - 0

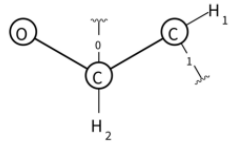




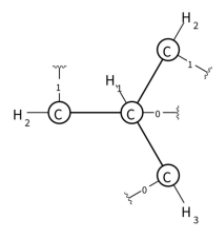
[#6X4H1][#6X4H1][#6X4H1]
0.991 0.000 0.217 2
1.000 - - 0



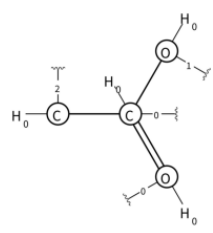
CCCC=CC
1.000 1.000 1.000 2
1.000 - - 0



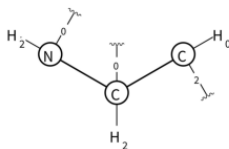
O[CX4H2][CX3H1]
1.000 1.000 1.000 2
1.000 - - 0



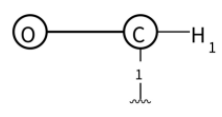
[CX4H1][CX4H3][CX4H2][CX4H2]
0.991 0.000 1.000 2
1.000 - - 0



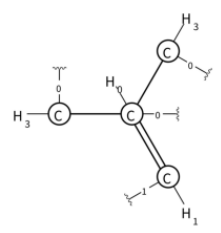
[CX3H0]=[OX1H0][OX2H0][CX3H0]
0.995 0.667 1.000 2
1.000 - - 0



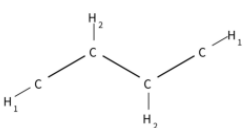
[CX4H2][NX3H2][CX3H0]
0.995 0.667 0.662 2
1.000 - - 0



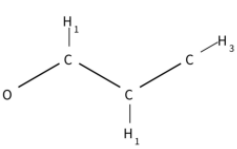
[CX3H](O)
1.000 1.000 1.000 2
1.000 - - 0



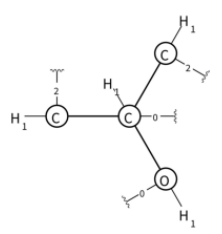
[CX3H0]=[CX3H1][CX4H3][CX4H3]
1.000 1.000 1.000 2
0.989 - - 0



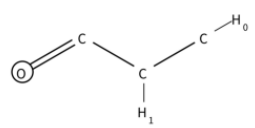
[#6H1][#6H2][#6H2][#6H1]
0.995 0.667 1.000 2
1.000 - - 0



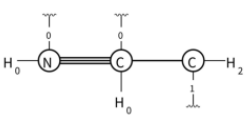
[#8][#6H1][#6H1][#6H3]
1.000 1.000 1.000 2
1.000 - - 0



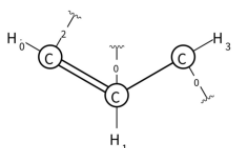
[CX4H1][OX2H1][CX4H1][CX4H1]
0.986 0.000 0.417 2
1.000 - - 0



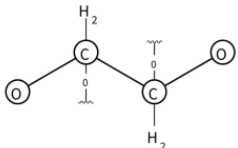
O=[#6][#6H][#6H0]
0.991 0.000 1.000 2
1.000 - - 0



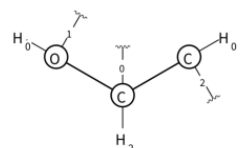
[CX2H0][#NX1H0][CX4H2]
1.000 1.000 1.000 2
1.000 - - 0



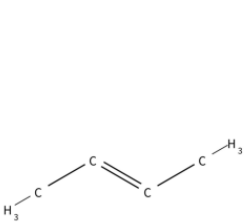
[CX3H1]=[CX3H0][CX4H3]
1.000 1.000 1.000 2
0.989 - - 0



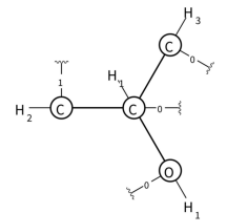
O[CX4H2][CX4H2]O
1.000 1.000 1.000 2
1.000 - - 0



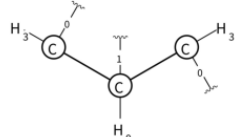
[CX4H2][OX2H0][CX3H0]
1.000 1.000 1.000 2
1.000 - - 0



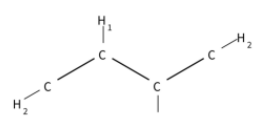
[#6H3][#6]=[#6][#6H3]
1.000 1.000 1.000 2
1.000 - - 0



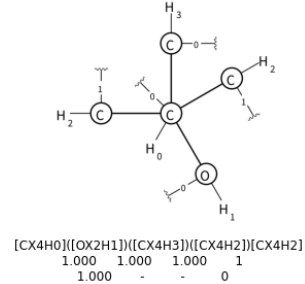
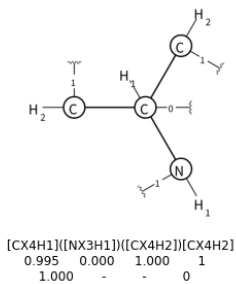
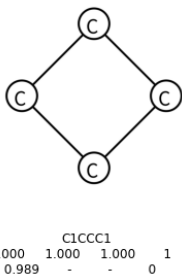
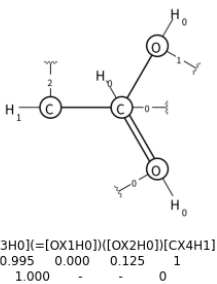
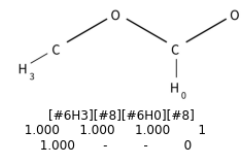
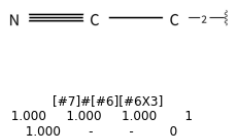
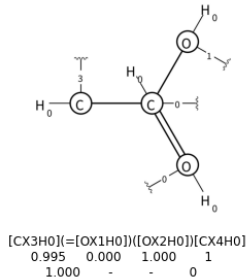
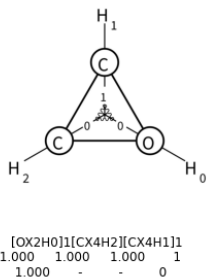
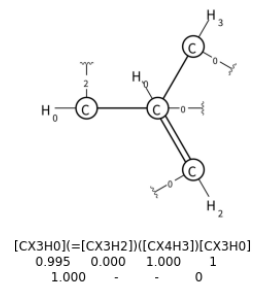
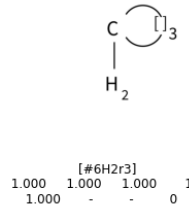
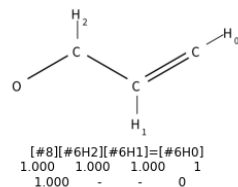
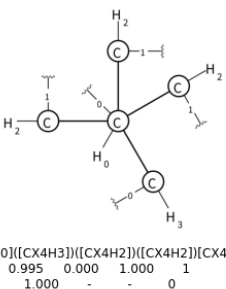
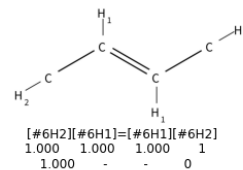
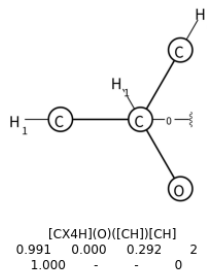
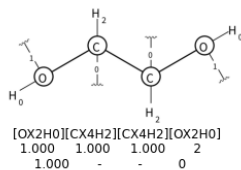
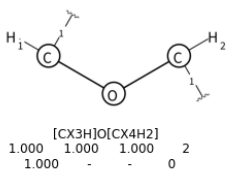
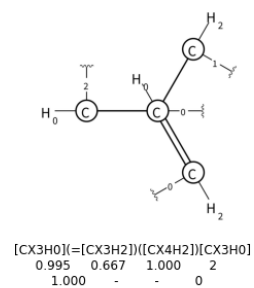
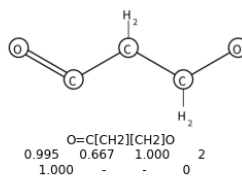
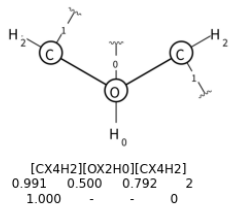
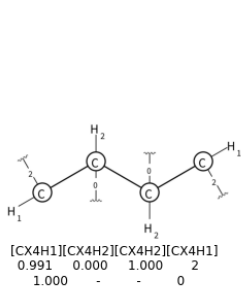
[CX4H1][OX2H1][CX4H3][CX4H2]
1.000 1.000 1.000 2
1.000 - - 0

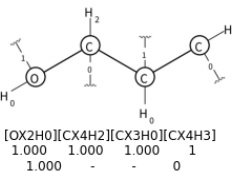
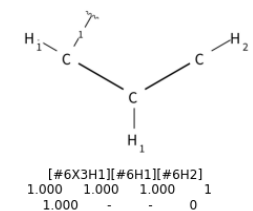
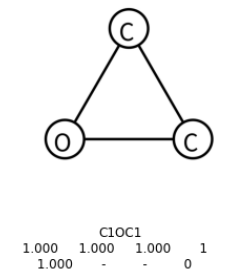
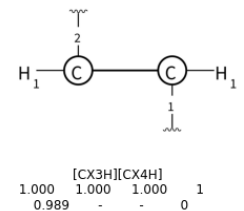
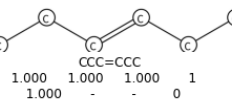
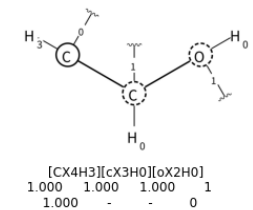
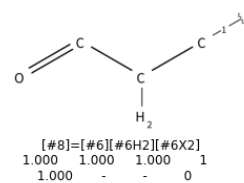
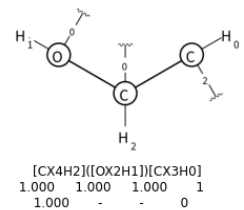
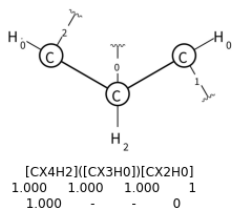
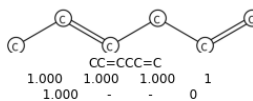
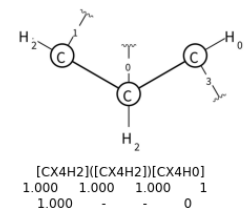
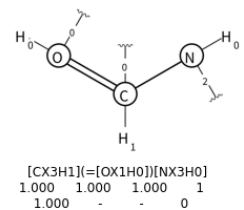
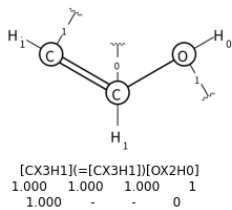
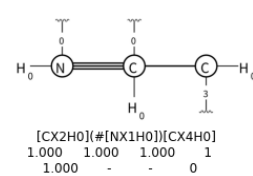
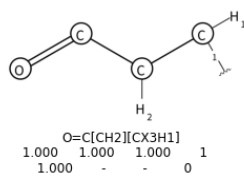
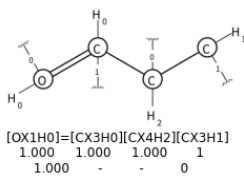
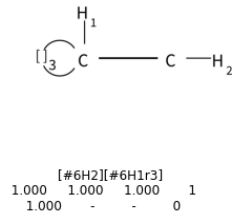
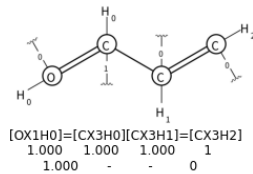
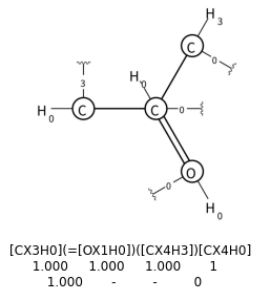
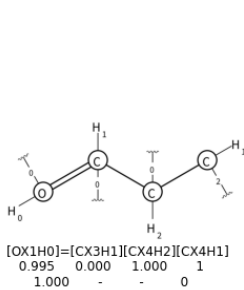


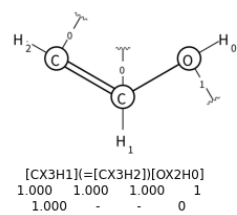
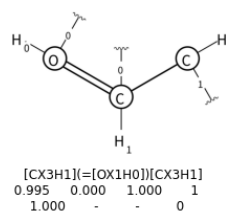
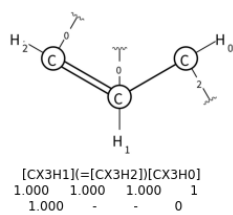
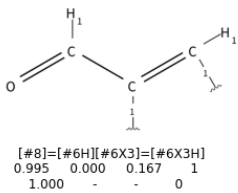
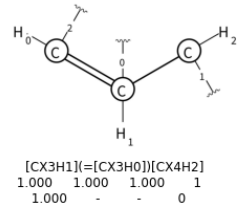
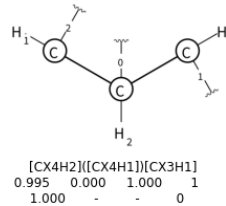
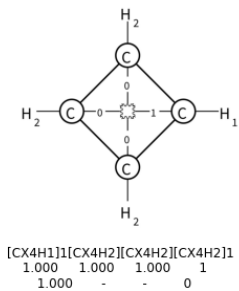
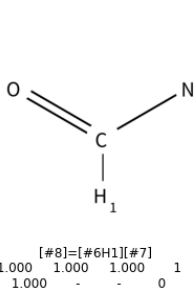
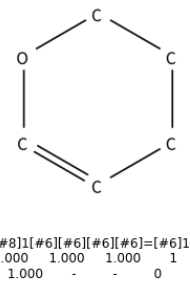
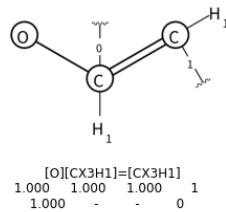
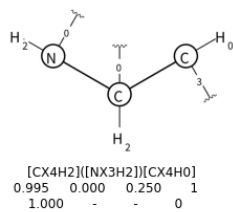
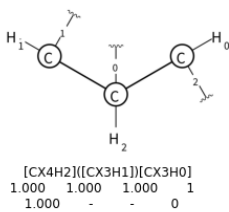
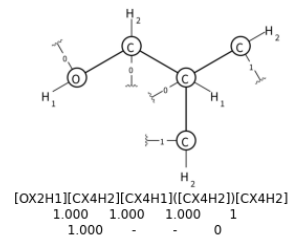
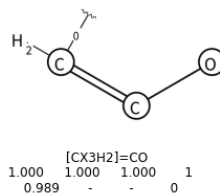
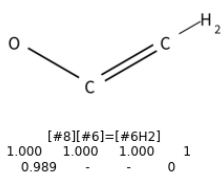
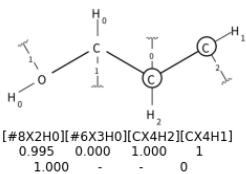
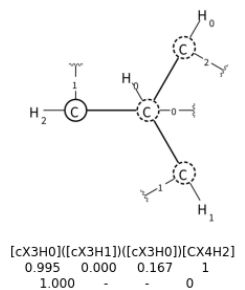
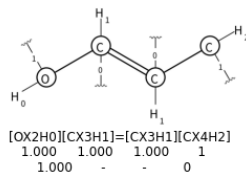
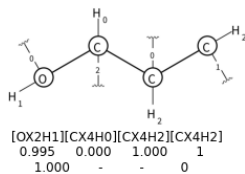
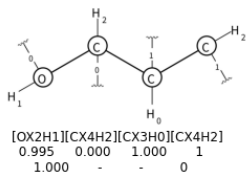
[CX4H3][CX3H0][CX4H3]
1.000 1.000 1.000 2
1.000 - - 0

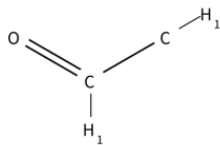


[#6H2][#6H1][#6H1][#6H2]
0.991 0.000 0.155 2
1.000 - - 0

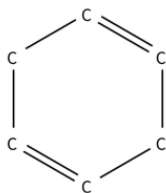




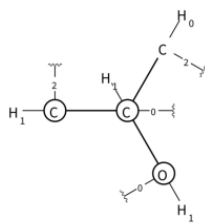




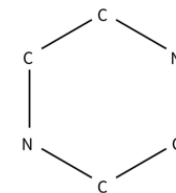
[#8]=[#6H1][#6H1]
0.995 0.000 0.167 1
1.000 - - 0



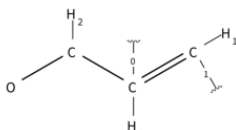
[#6]1[#6]=[#6][#6][#6]=[#6]1
1.000 1.000 1.000 1
1.000 - - 0



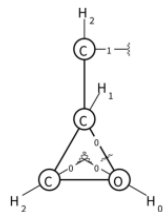
[OX2H1][CX4H1][#6X3H0][CX4H1]
1.000 1.000 1.000 1
1.000 - - 0



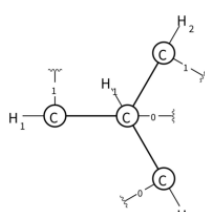
[#6]1[#6][#7][#6][#6][#7]1
1.000 1.000 1.000 1
1.000 - - 0



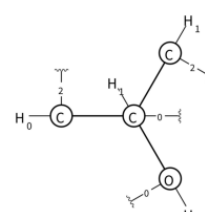
[#8][#6H2][#6X3H]=[#6X3H]
1.000 1.000 1.000 1
1.000 - - 0



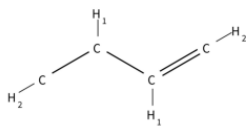
[OX2H0]1[CX4H2][CX4H1]1[CX4H2]
1.000 1.000 1.000 1
1.000 - - 0



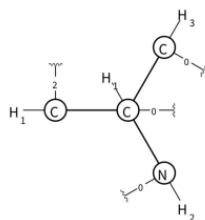
[CX4H1][CX4H3][CX4H2][CX3H1]
1.000 1.000 1.000 1
1.000 - - 0



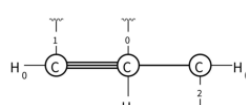
[CX4H1][OX2H1][CX4H1][CX3H0]
1.000 1.000 1.000 1
1.000 - - 0



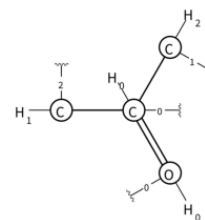
[#6H2][#6H1][#6H1]=[#6H2]
1.000 1.000 1.000 1
0.989 - - 0



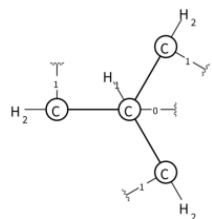
[CX4H1][NX3H2][CX4H3][CX4H1]
1.000 1.000 1.000 1
1.000 - - 0



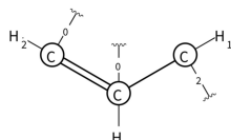
[CX2H0][#CX2H0][CX3H0]
1.000 1.000 1.000 1
1.000 - - 0



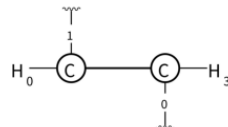
[CX3H0][OX1H0][CX4H2][CX4H1]
1.000 1.000 1.000 1
1.000 - - 0



[CX4H1][CX4H2][CX4H2][CX4H2]
1.000 1.000 1.000 1
1.000 - - 0



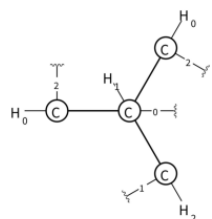
[CX3H1][CX3H2][CX4H1]
1.000 1.000 1.000 1
0.989 - - 0



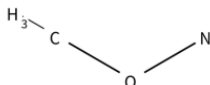
[CX4H3][CX2H0]
1.000 1.000 1.000 1
1.000 - - 0



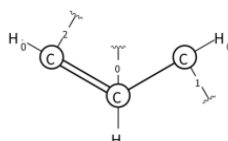
[#6X3][#6][#6][#6H3]
1.000 1.000 1.000 1
1.000 - - 0



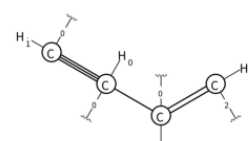
[CX4H1][CX4H2][CX3H0][CX3H0]
0.995 0.000 1.000 1
1.000 - - 0



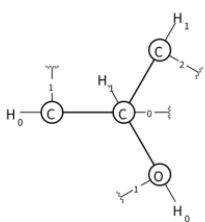
[#6H3][#8][#7]
1.000 - - 0
1.000 - - 0



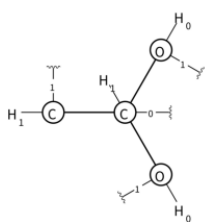
[CX3H1][CX3H0][CX2H0]
1.000 - - 0
1.000 - - 0



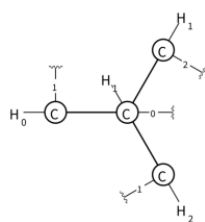
[CX2H1][CX2H0][CX3H1][CX3H0]
1.000 - - 0
1.000 - - 0



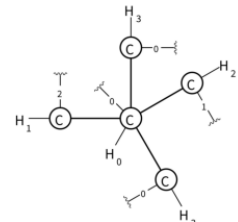
[CX4H1][OX2H0][CX4H1][CX2H0]
 1.000 - - 0
 1.000 - - 0



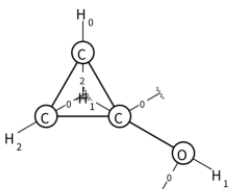
[CX4H1][OX2H0][OX2H0][CX3H1]
 1.000 - - 0
 1.000 - - 0



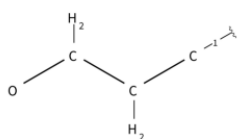
[CX4H1][CX4H2][CX4H1][CX2H0]
 1.000 - - 0
 1.000 - - 0



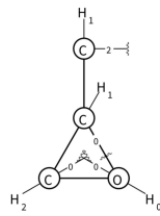
[CX4H0][CX4H3][CX4H3][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



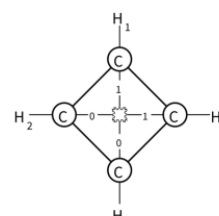
[OX2H1][CX4H1][CX4H2][CX4H0]1
 1.000 - - 0
 1.000 - - 0



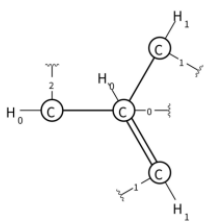
[#8][#6H2][#6H2][#6X2]
 1.000 - - 0
 1.000 - - 0



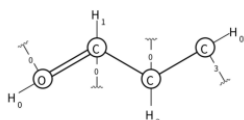
[OX2H0]1[CX4H2][CX4H1]1[CX4H1]
 1.000 - - 0
 1.000 - - 0



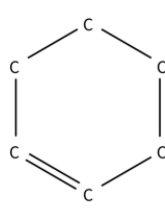
[CX4H1]1[CX4H2][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



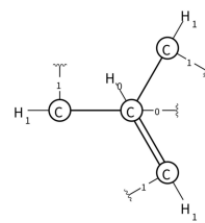
[CX3H0][=CX3H1][CX3H1][CX3H0]
 1.000 - - 0
 1.000 - - 0



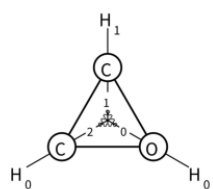
[OX1H0][CX3H1][CX4H2][CX4H0]
 1.000 - - 0
 1.000 - - 0



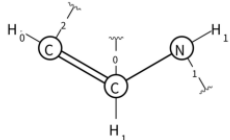
[#6]1[#6][#6]=[#6][#6]=[#6]1
 1.000 - - 0
 1.000 - - 0



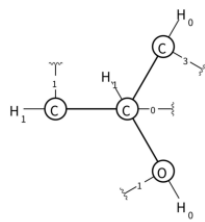
[CX3H0][=CX3H1][CX3H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



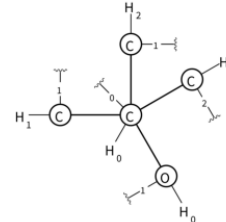
[OX2H0]1[CX4H0][CX4H1]1
 1.000 - - 0
 1.000 - - 0



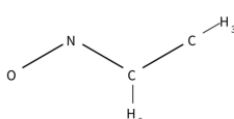
[CX3H1][=CX3H0][NX3H1]
 1.000 - - 0
 1.000 - - 0



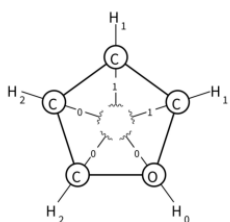
[CX4H1][OX2H0][CX4H0][CX3H1]
 1.000 - - 0
 1.000 - - 0



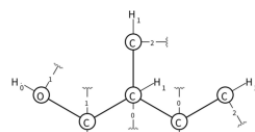
[CX4H0][OX2H0][CX4H2][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



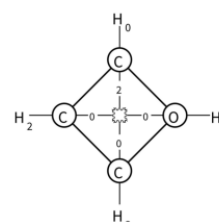
[#8][#7][#6H0][#6H3]
 1.000 - - 0
 1.000 - - 0



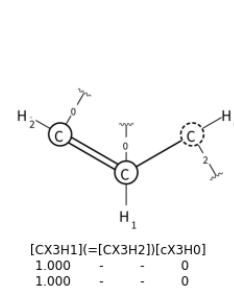
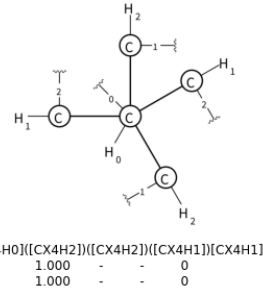
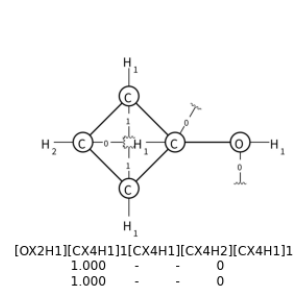
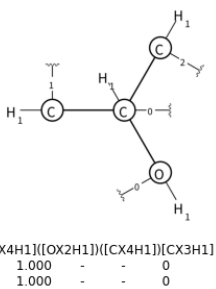
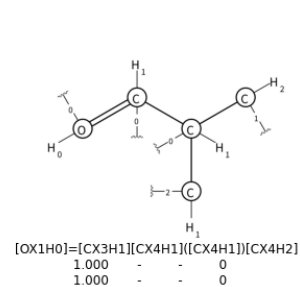
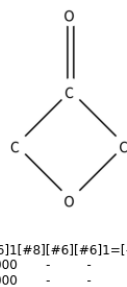
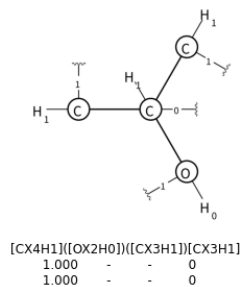
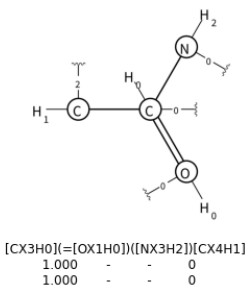
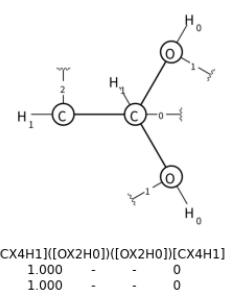
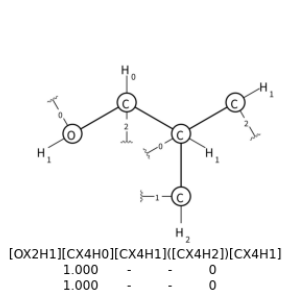
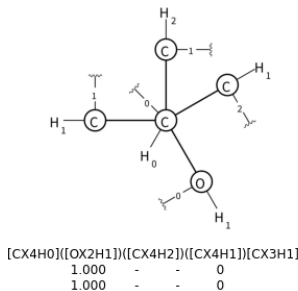
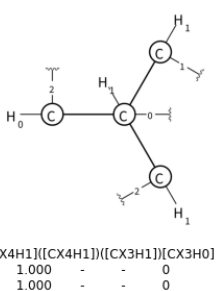
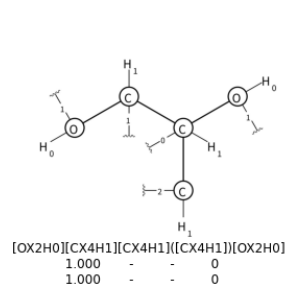
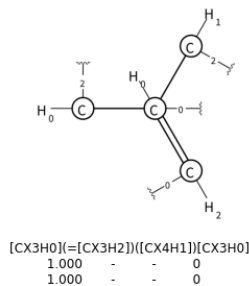
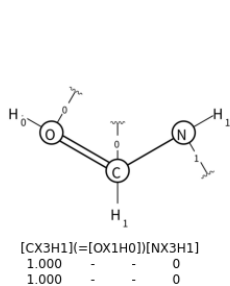
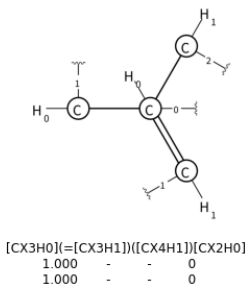
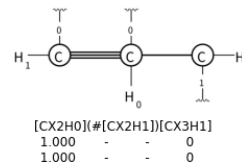
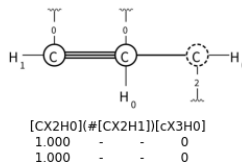
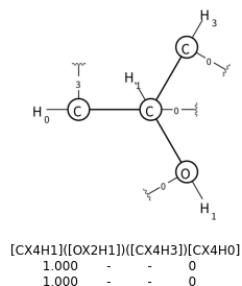
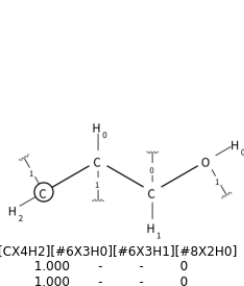
[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1
 1.000 - - 0
 1.000 - - 0

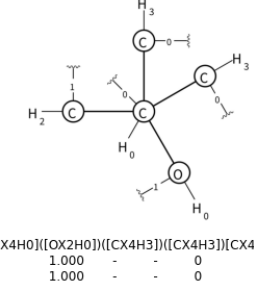
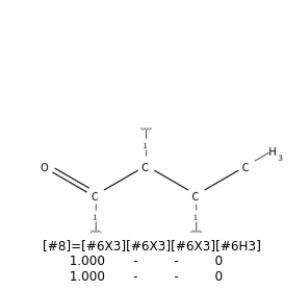
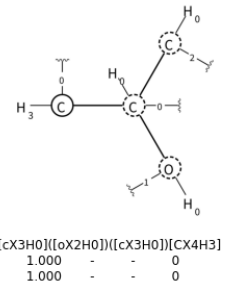
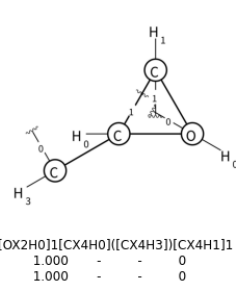
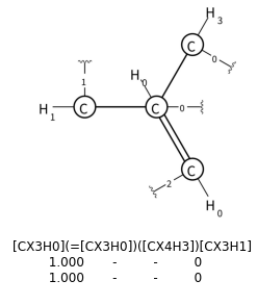
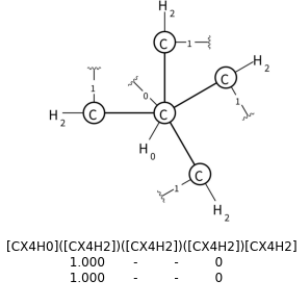
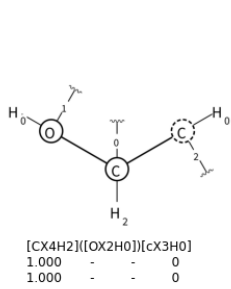
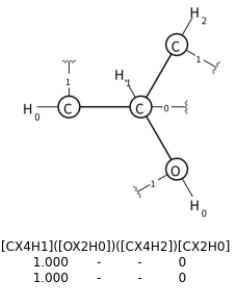
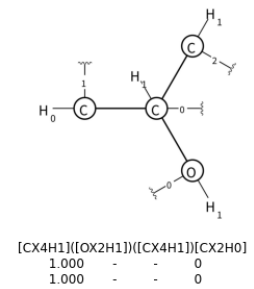
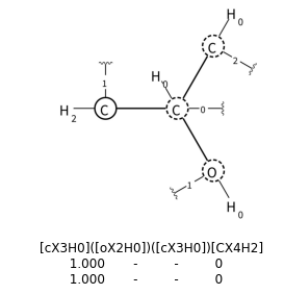
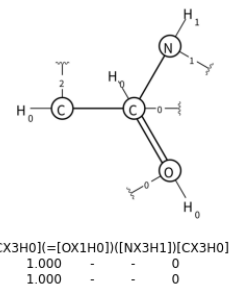
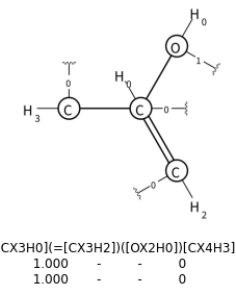
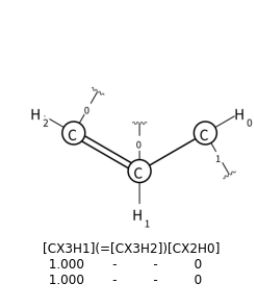
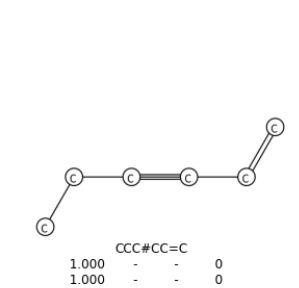
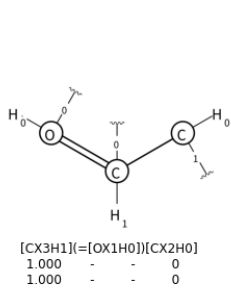
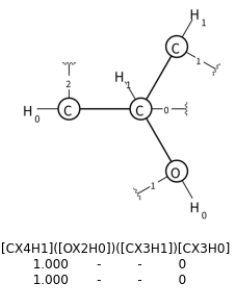
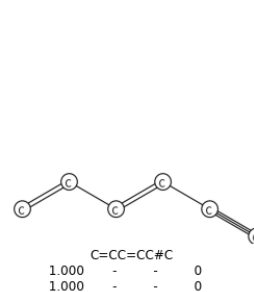
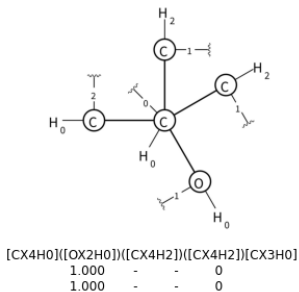
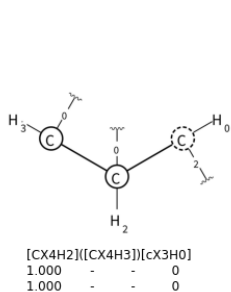
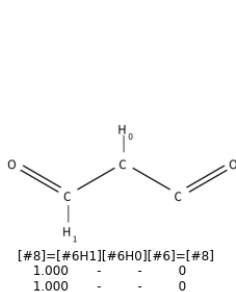


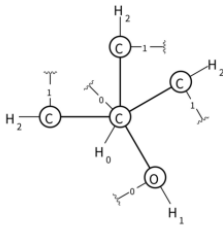
[OX2H0][CX4H1][CX4H1][CX4H2][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



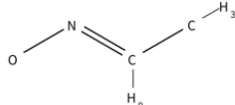
[OX2H0]1[CX4H2][CX4H2][CX4H0]1
 1.000 - - 0
 1.000 - - 0



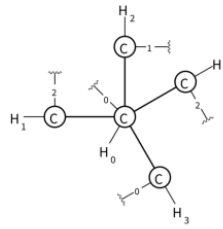




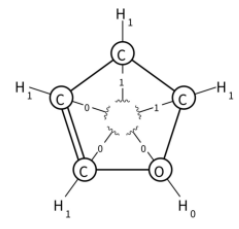
[CX4H0]([OX2H1])([CX4H2])([CX4H2])[CX4H2]
 1.000 - - 0
 1.000 - - 0



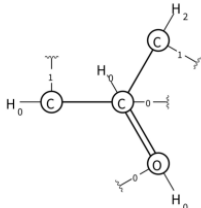
[#8][#7]=[#6H0][#6H3]
 1.000 - - 0
 1.000 - - 0



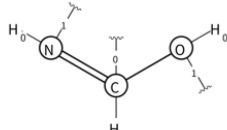
[CX4H0]([CX4H3])([CX4H2])([CX4H1])(CX4H1]
 1.000 - - 0
 1.000 - - 0



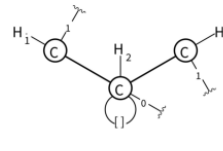
[OX2H0]1[CX3H1]=[CX3H1][CX4H1][CX4H11]
 1.000 - - 0
 1.000 - - 0



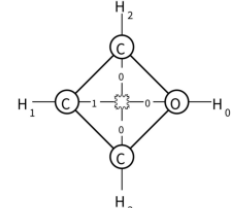
[CX3H0](=[OX1H0])([CX4H2])(CX2H0]
 1.000 - - 0
 1.000 - - 0



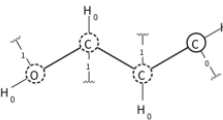
[CX3H1](=[NX2H0])([OX2H0]
 1.000 - - 0
 1.000 - - 0



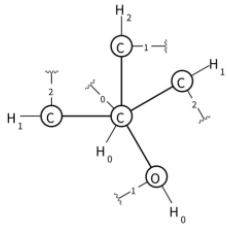
[CX3H1][CX4H2r0][CX3H1]
 1.000 - - 0
 1.000 - - 0



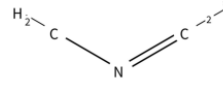
[OX2H0]1[CX4H2][CX4H1][CX4H2]1
 1.000 - - 0
 1.000 - - 0



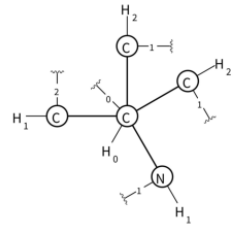
[OX2H0][CX3H0][CX3H0][CX4H3]
 1.000 - - 0
 1.000 - - 0



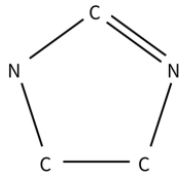
[CX4H0]([OX2H0])([CX4H2])([CX4H1])(CX4H1]
 1.000 - - 0
 1.000 - - 0



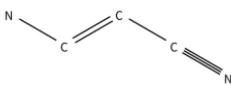
[#6H2][#7]=[#6X3]
 1.000 - - 0
 1.000 - - 0



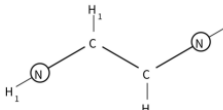
[CX4H0]([NX3H1])([CX4H2])([CX4H2])(CX4H1]
 1.000 - - 0
 1.000 - - 0



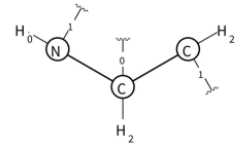
[#6]1[#6][#7][#6]=[#7]1
 1.000 - - 0
 1.000 - - 0



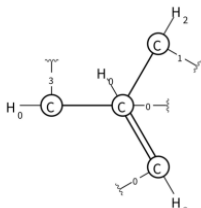
[#7][#6]=[#6][#6][#7]
 1.000 - - 0
 1.000 - - 0



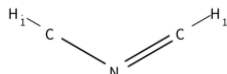
[NH1][#6H1][#6H1][NH1]
 1.000 - - 0
 1.000 - - 0



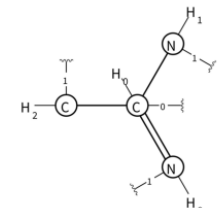
[CX4H2]([NX2H0])(CX4H2]
 1.000 - - 0
 1.000 - - 0



[CX3H0](=[CX3H2])([CX4H2])(CX4H0]
 1.000 - - 0
 1.000 - - 0



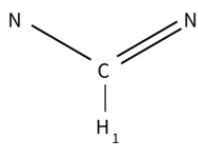
[#6H1][#7]=[#6H1]
 1.000 - - 0
 1.000 - - 0



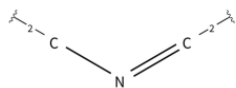
[CX3H0](=[NX2H0])([NX3H1])(CX4H2]
 1.000 - - 0
 1.000 - - 0



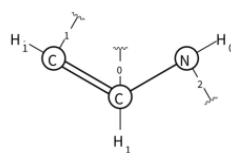
[CX3H1](=[NX2H0])[NX3H1]
 1.000 - - 0
 1.000 - - 0



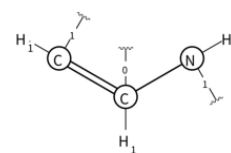
[#7][#6H1]=[#7]
 1.000 - - 0
 1.000 - - 0



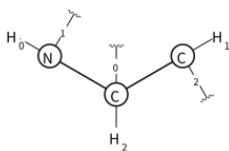
[#6X3][#7]=[#6X3]
 1.000 - - 0
 1.000 - - 0



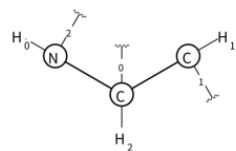
[CX3H1](=[CX3H1])[NX3H0]
 1.000 - - 0
 1.000 - - 0



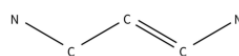
[CX3H1](=[CX3H1])[NX3H1]
 1.000 - - 0
 1.000 - - 0



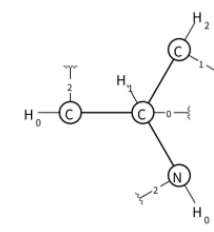
[CX4H2]([NX2H0])[CX4H1]
 1.000 - - 0
 1.000 - - 0



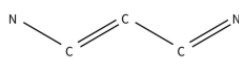
[CX4H2]([NX3H0])[CX3H1]
 1.000 - - 0
 1.000 - - 0



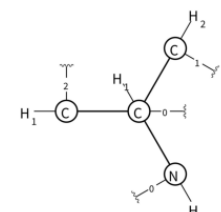
[#7][#6][#6]=[#6][#7]
 1.000 - - 0
 1.000 - - 0



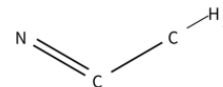
[CX4H1]([NX3H0])([CX4H2])[CX3H0]
 1.000 - - 0
 1.000 - - 0



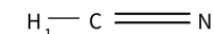
[#7][#6]=[#6][#6]=[#7]
 1.000 - - 0
 1.000 - - 0



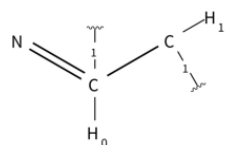
[CX4H1]([NX3H2])([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



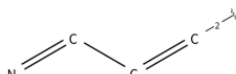
[#7]=[#6][#6H3]
 1.000 - - 0
 1.000 - - 0



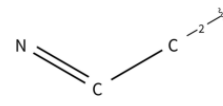
[#7]=[#6H1]
 1.000 - - 0
 1.000 - - 0



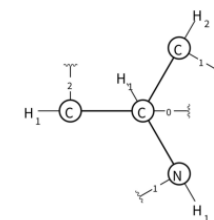
[#7]=[#6X3H0][#6X3H1]
 1.000 - - 0
 1.000 - - 0



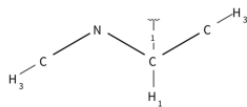
[#7]=[#6][#6]=[#6X3]
 1.000 - - 0
 1.000 - - 0



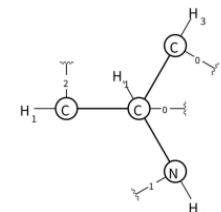
[#7]=[#6][#6X3]
 1.000 - - 0
 1.000 - - 0



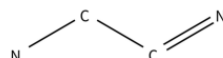
[CX4H1]([NX3H1])([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



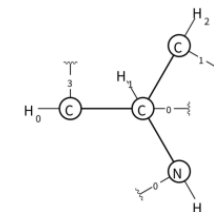
[#6H3][#7][#6X4H1][#6H3]
 1.000 - - 0
 1.000 - - 0



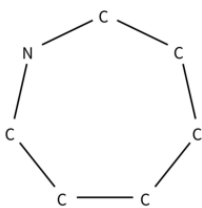
[CX4H1]([NX3H1])([CX4H3])[CX4H1]
 1.000 - - 0
 1.000 - - 0



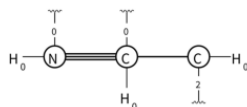
[#7][#6][#6]=[#7]
 1.000 - - 0
 1.000 - - 0



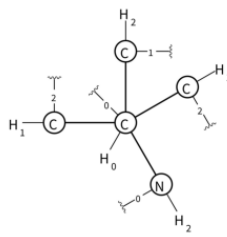
[CX4H1]([NX3H2])([CX4H2])[CX4H0]
 1.000 - - 0
 1.000 - - 0



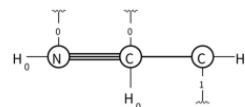
[#6][#6][#6][#7][#6][#6][#6]1
 1.000 - - 0
 1.000 - - 0



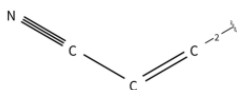
[CX2H0][#(NX1H0)][CX3H0]
 1.000 - - 0
 1.000 - - 0



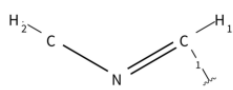
[CX4H0][!(NX3H2)][!(CX4H2)][!(CX4H1)][CX4H1]
 1.000 - - 0
 1.000 - - 0



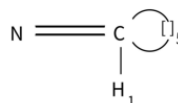
[CX2H0][#(NX1H0)][CX3H1]
 1.000 - - 0
 1.000 - - 0



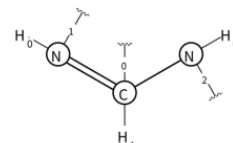
[#7][#6][#6]=[#6X3]
 1.000 - - 0
 1.000 - - 0



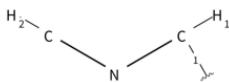
[#6H2][#7]=[#6X3H1]
 1.000 - - 0
 1.000 - - 0



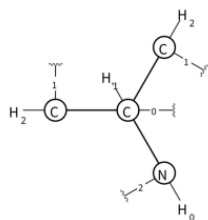
[#6H1r5]=[#7]
 1.000 - - 0
 1.000 - - 0



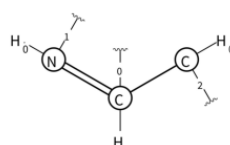
[CX3H1][!(NX2H0)][NX3H0]
 1.000 - - 0
 1.000 - - 0



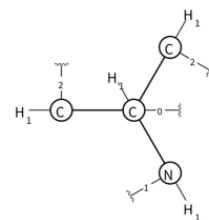
[#6H2][#7][#6X3H1]
 1.000 - - 0
 1.000 - - 0



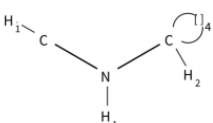
[CX4H1][!(NX3H0)][!(CX4H2)][CX4H2]
 1.000 - - 0
 1.000 - - 0



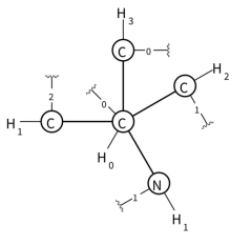
[CX3H1][!(NX2H0)][CX3H0]
 1.000 - - 0
 1.000 - - 0



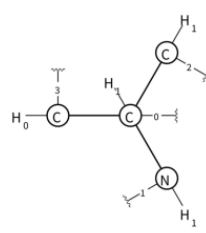
[CX4H1][!(NX3H1)][!(CX4H1)][CX4H1]
 1.000 - - 0
 1.000 - - 0



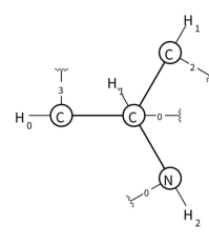
[#6H1][#7H1][#6H2r4]
 1.000 - - 0
 1.000 - - 0



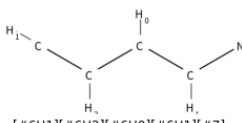
[CX4H0][!(NX3H1)][!(CX4H3)][!(CX4H2)][CX4H1]
 1.000 - - 0
 1.000 - - 0



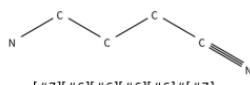
[CX4H1][!(NX3H1)][!(CX4H1)][CX4H0]
 1.000 - - 0
 1.000 - - 0



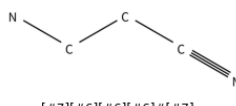
[CX4H1][!(NX3H2)][!(CX4H1)][CX4H0]
 1.000 - - 0
 1.000 - - 0



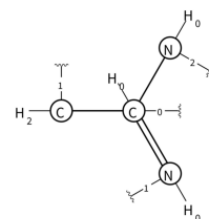
[#6H1][#6H2][#6H0][#6H1][#7]
 1.000 - - 0
 1.000 - - 0



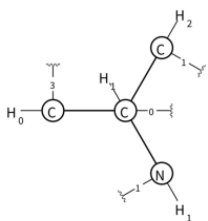
[#7][#6][#6][#6][#6][#7]
 1.000 - - 0
 1.000 - - 0



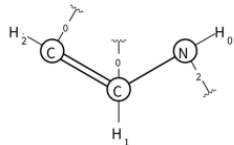
[#7][#6][#6][#6][#7]
 1.000 - - 0
 1.000 - - 0



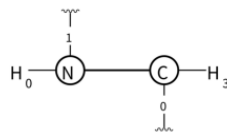
[CX3H0][!(NX2H0)][!(NX3H0)][CX4H2]
 1.000 - - 0
 1.000 - - 0



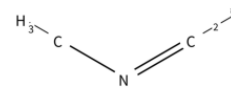
[CX4H1]([NX3H1])([CX4H2])[CX4H0]
 1.000 - - 0
 1.000 - - 0



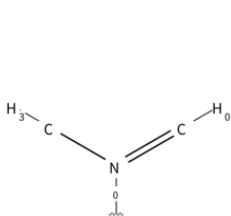
[CX3H1](=[CX3H2])[NX3H0]
 1.000 - - 0
 1.000 - - 0



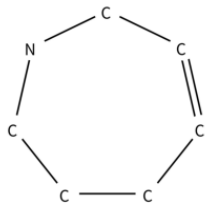
[CX4H3][NX2H0]
 1.000 - - 0
 1.000 - - 0



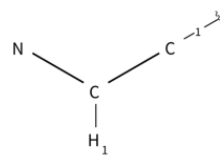
[#6H3][#7]=[#6X3]
 1.000 - - 0
 1.000 - - 0



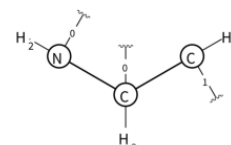
[#6H3][#7X2]=[#6H0]
 1.000 - - 0
 1.000 - - 0



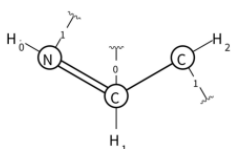
[#6]1[#6][#6][#7][#6][#6]=[#6]1
 1.000 - - 0
 1.000 - - 0



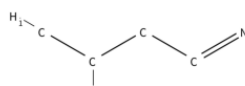
[#7][#6H1][#6X2]
 1.000 - - 0
 1.000 - - 0



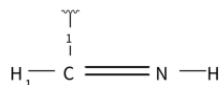
[CX4H2]([NX3H2])[CX3H1]
 1.000 - - 0
 1.000 - - 0



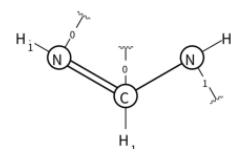
[CX3H1](=[NX2H0])[CX4H2]
 1.000 - - 0
 1.000 - - 0



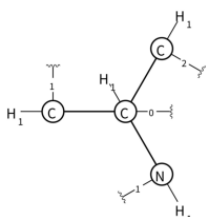
[#6H1][#6H2][#6][#6]=[#7]
 1.000 - - 0
 1.000 - - 0



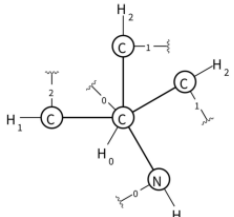
[#7H]=[#6X3H1]
 1.000 - - 0
 1.000 - - 0



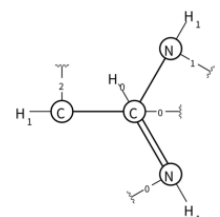
[CX3H1](=[NX2H1])[NX3H1]
 1.000 - - 0
 1.000 - - 0



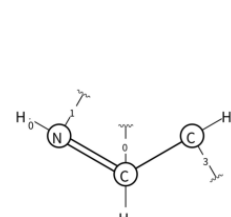
[CX4H1]([NX3H1])([CX4H1])[CX3H1]
 1.000 - - 0
 1.000 - - 0



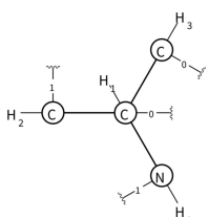
[CX4H0]([NX3H2])([CX4H2])([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



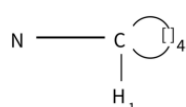
[CX3H0](=[NX2H1])([NX3H1])[CX4H1]
 1.000 - - 0
 1.000 - - 0



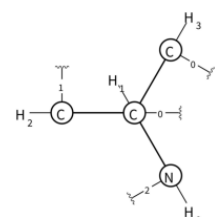
[CX3H1](=[NX2H0])[CX4H0]
 1.000 - - 0
 1.000 - - 0



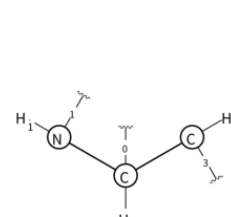
[CX4H1]([NX3H1])([CX4H3])[CX4H2]
 1.000 - - 0
 1.000 - - 0



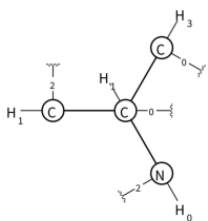
[#6H1r4][#7]
 1.000 - - 0
 1.000 - - 0



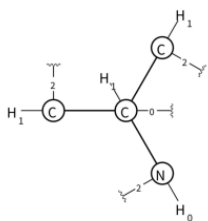
[CX4H1]([NX3H0])([CX4H3])[CX4H2]
 1.000 - - 0
 1.000 - - 0



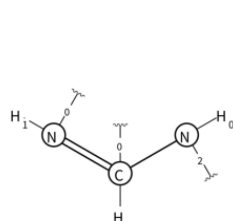
[CX4H2]([NX3H1])[CX4H0]
 1.000 - - 0
 1.000 - - 0



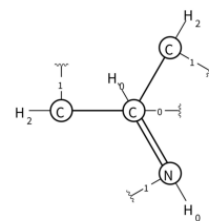
[CX4H1]([NX3H0])([CX4H3])[CX4H1]
 1.000 - - 0
 1.000 - - 0



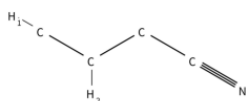
[CX4H1]([NX3H0])([CX4H1])[CX4H1]
 1.000 - - 0
 1.000 - - 0



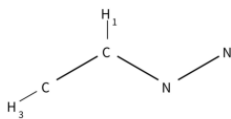
[CX3H1](=[NX2H1])([NX3H0])
 1.000 - - 0
 1.000 - - 0



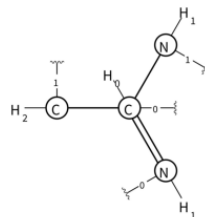
[CX3H0](=[NX2H0])([CX4H2])[CX4H2]
 1.000 - - 0
 1.000 - - 0



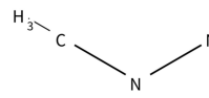
[#6H1][#6H2][#6][#6][#7]
 1.000 - - 0
 1.000 - - 0



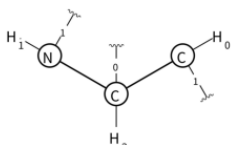
[#6H3][#6H1][#7][#7]
 1.000 - - 0
 1.000 - - 0



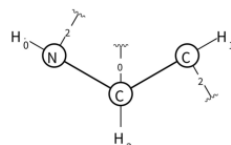
[CX3H0](=[NX2H1])([NX3H1])[CX4H2]
 1.000 - - 0
 1.000 - - 0



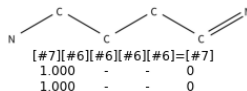
[#6H3][#7][#7]
 1.000 - - 0
 1.000 - - 0



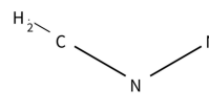
[CX4H2]([NX3H1])[CX2H0]
 1.000 - - 0
 1.000 - - 0



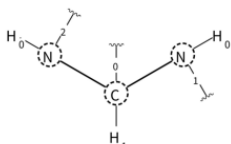
[CX4H2]([NX3H0])[CX4H1]
 1.000 - - 0
 1.000 - - 0



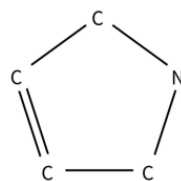
[#7][#6][#6][#6][#6]=[#7]
 1.000 - - 0
 1.000 - - 0



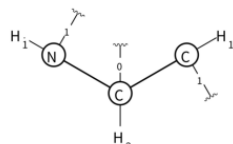
[#6H2][#7][#7]
 1.000 - - 0
 1.000 - - 0



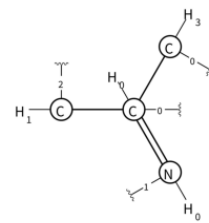
[cX3H1]([nX3H0])(nX2H0)
 1.000 - - 0
 1.000 - - 0



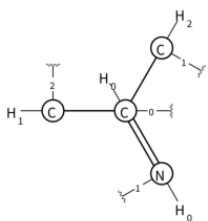
[#6]1[#6]=[#6][#6][#7]1
 1.000 - - 0
 1.000 - - 0



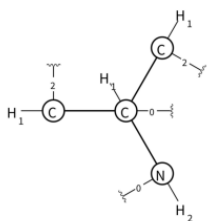
[CX4H2]([NX3H1])[CX3H1]
 1.000 - - 0
 1.000 - - 0



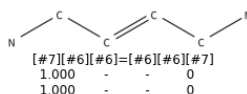
[CX3H0](=[NX2H0])([CX4H3])[CX4H1]
 1.000 - - 0
 1.000 - - 0



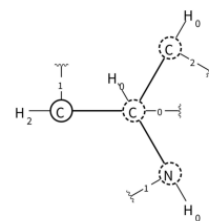
[CX3H0](=[NX2H0])([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



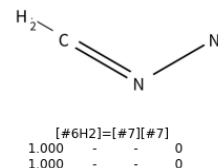
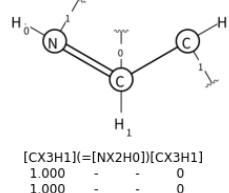
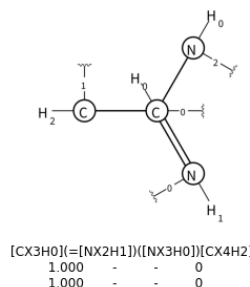
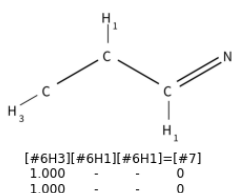
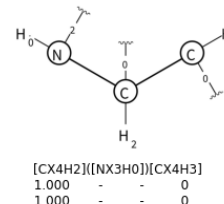
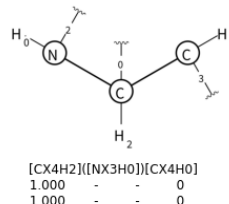
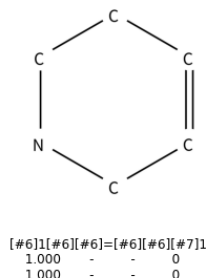
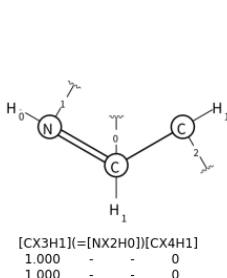
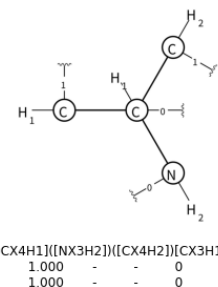
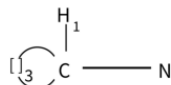
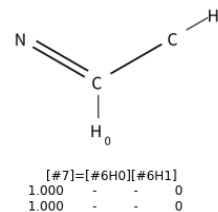
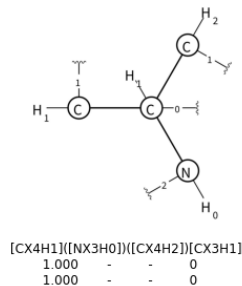
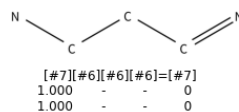
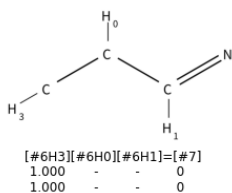
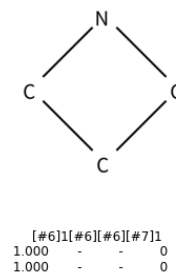
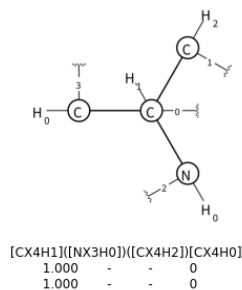
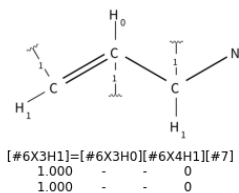
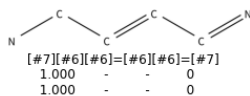
[CX4H1]([NX3H2])([CX4H1])[CX4H1]
 1.000 - - 0
 1.000 - - 0

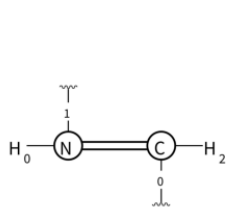


[#7][#6][#6]=[#6][#6][#7]
 1.000 - - 0
 1.000 - - 0

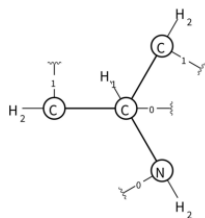


[cX3H0]([nX2H0])([CX3H0])[CX4H2]
 1.000 - - 0
 1.000 - - 0

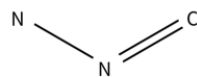




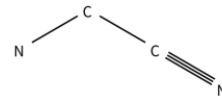
[CX3H2]=[NX2H0]
 1.000 - - 0
 1.000 - - 0



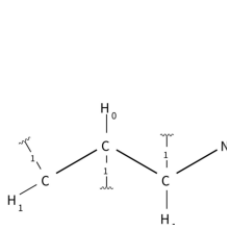
[CX4H1]([NX3H2])([CX4H2])([CX4H2])
 1.000 - - 0
 1.000 - - 0



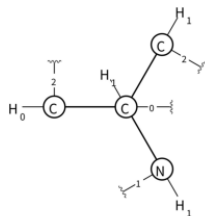
[#7][#7]=[#6]
 1.000 - - 0
 1.000 - - 0



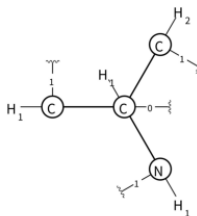
[#7][#6][#6][#7]
 1.000 - - 0
 1.000 - - 0



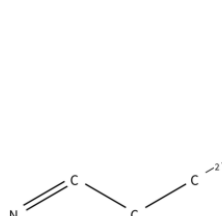
[#6X3H1][#6X3H0][#6X4H1][#7]
 1.000 - - 0
 1.000 - - 0



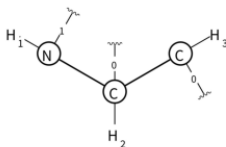
[CX4H1]([NX3H1])([CX4H1])([CX3H0])
 1.000 - - 0
 1.000 - - 0



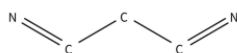
[CX4H1]([NX3H1])([CX4H2])([CX3H1])
 1.000 - - 0
 1.000 - - 0



[#7]=[#6][#6][#6X3]
 1.000 - - 0
 1.000 - - 0



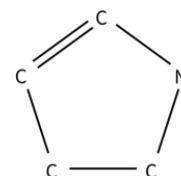
[CX4H2]([NX3H1])([CX4H3])
 1.000 - - 0
 1.000 - - 0



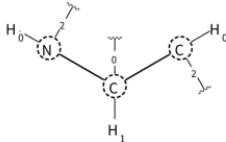
[#7]=[#6][#6][#6]=[#7]
 1.000 - - 0
 1.000 - - 0



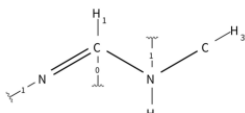
[#7][#6]=[#6][#6][#6]=[#7]
 1.000 - - 0
 1.000 - - 0



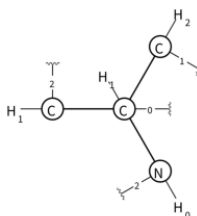
[#6][#6][#6]=[#6][#7]1
 1.000 - - 0
 1.000 - - 0



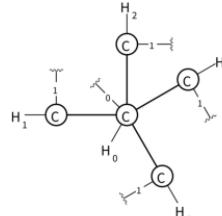
[CX3H1]([NX3H0])([CX3H0])
 1.000 - - 0
 1.000 - - 0



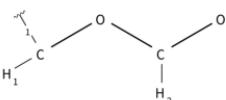
[#7X2]=[#6X3H1][#7X3H0][#6H3]
 1.000 - - 0
 1.000 - - 0



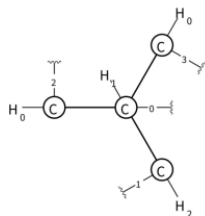
[CX4H1]([NX3H0])([CX4H2])([CX4H1])
 1.000 - - 0
 1.000 - - 0



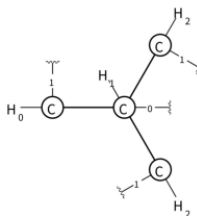
[CX4H0]([CX4H2])([CX4H2])([CX4H2])([CX3H1])
 1.000 - - 0
 1.000 - - 0



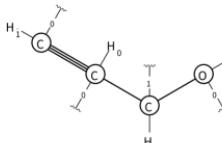
[#6X3H1][#8][#6H2][#8]
 1.000 - - 0
 1.000 - - 0



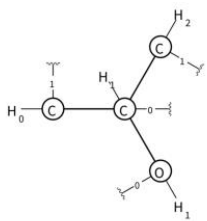
[CX4H1]([CX4H2])([CX4H0])([CX3H0])
 1.000 - - 0
 1.000 - - 0



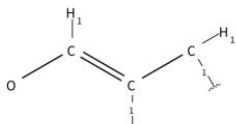
[CX4H1]([CX4H2])([CX4H2])([CX2H0])
 1.000 - - 0
 1.000 - - 0



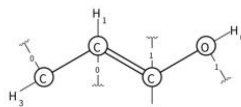
[CX2H1][CX2H0][CX4H1][OX2H1]
 1.000 - - 0
 1.000 - - 0



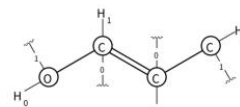
[CX4H1][OX2H1][CX4H2][CX2H0]
 1.000 - - 0
 1.000 - - 0



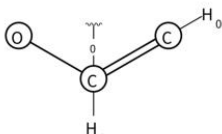
[#8][#6H]=[#6X3][#6X3H]
 1.000 - - 0
 1.000 - - 0



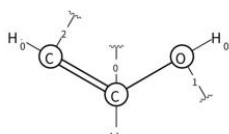
[CX4H3][CX3H1]=[CX3H0][OX2H0]
 1.000 - - 0
 1.000 - - 0



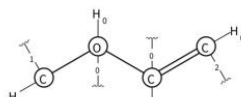
[OX2H0][CX3H1]=[CX3H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



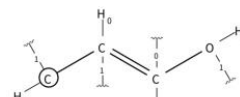
O[CX3H]=[CH0]
 1.000 - - 0
 1.000 - - 0



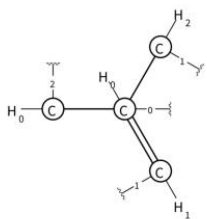
[CX3H1]=[CX3H0][OX2H0]
 1.000 - - 0
 1.000 - - 0



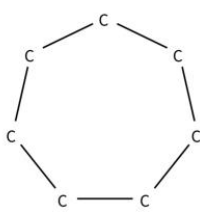
[CX4H2][OX2H0][CX3H1]=[CX3H0]
 1.000 - - 0
 1.000 - - 0



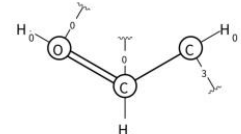
[CX4H2][#6X3H0]=[#6X3H1][#8X2H0]
 1.000 - - 0
 1.000 - - 0



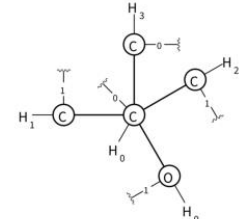
[CX3H0]=[CX3H1][CX4H2][CX3H0]
 1.000 - - 0
 1.000 - - 0



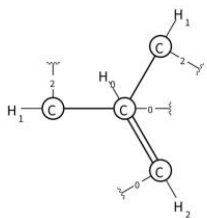
[#6][#6][#6][#6][#6][#6]
 1.000 - - 0
 1.000 - - 0



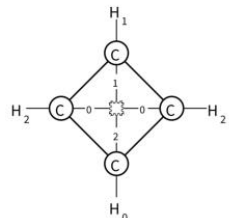
[CX3H1]=[OX1H0][CX4H0]
 1.000 - - 0
 1.000 - - 0



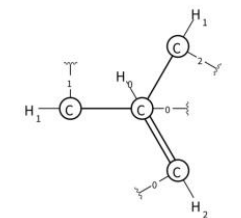
[CX4H0][OX2H0][CX4H3][CX4H2][CX3H1]
 1.000 - - 0
 1.000 - - 0



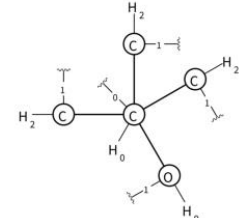
[CX3H0]=[CX3H2][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



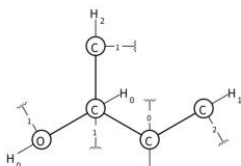
[CX4H2][CX4H0][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



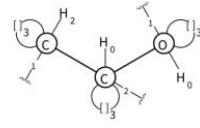
[CX3H0]=[CX3H2][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



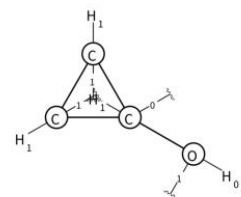
[CX4H0][OX2H0][CX4H2][CX4H2][CX4H2]
 1.000 - - 0
 1.000 - - 0



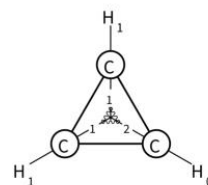
[OX2H0][CX4H0][CX4H2][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



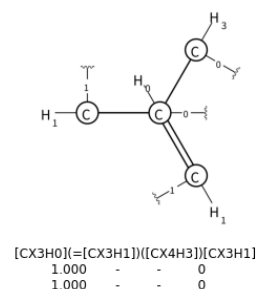
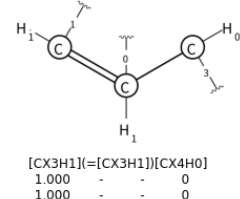
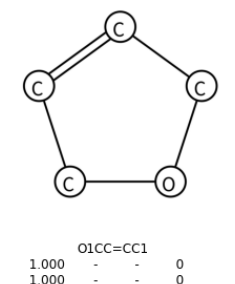
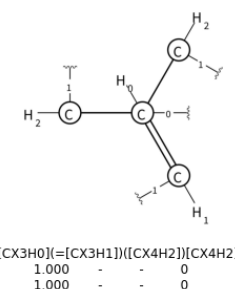
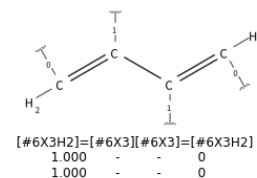
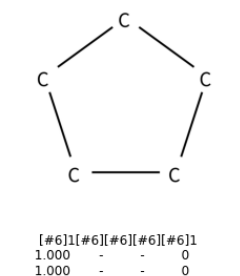
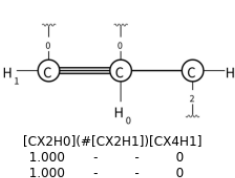
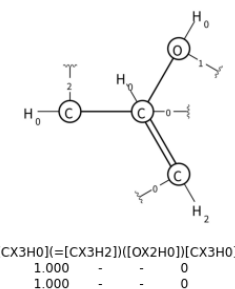
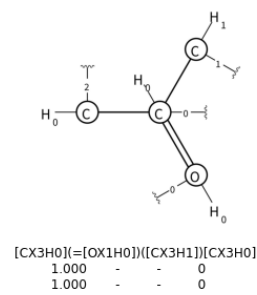
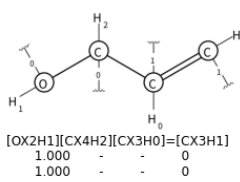
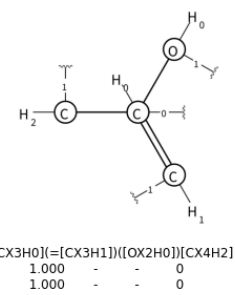
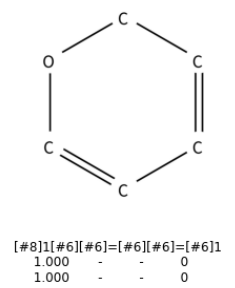
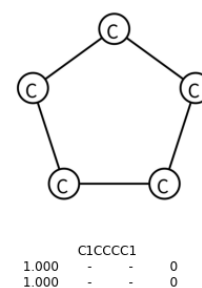
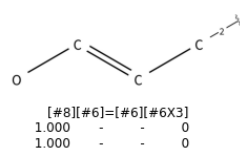
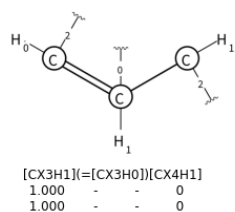
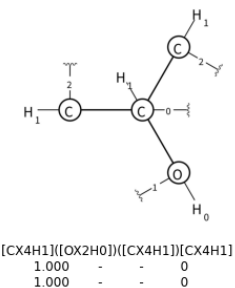
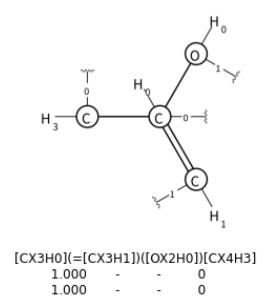
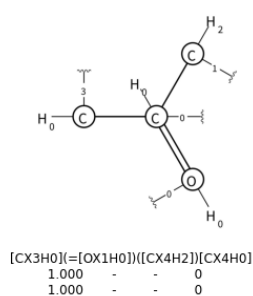
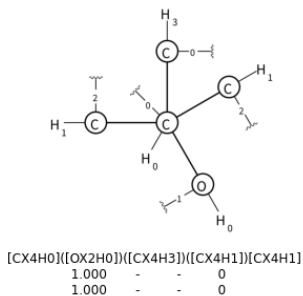
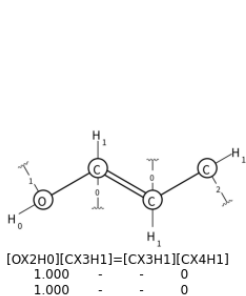
[CX4H2r3][CX4H0r3][OX2H0r3]
 1.000 - - 0
 1.000 - - 0

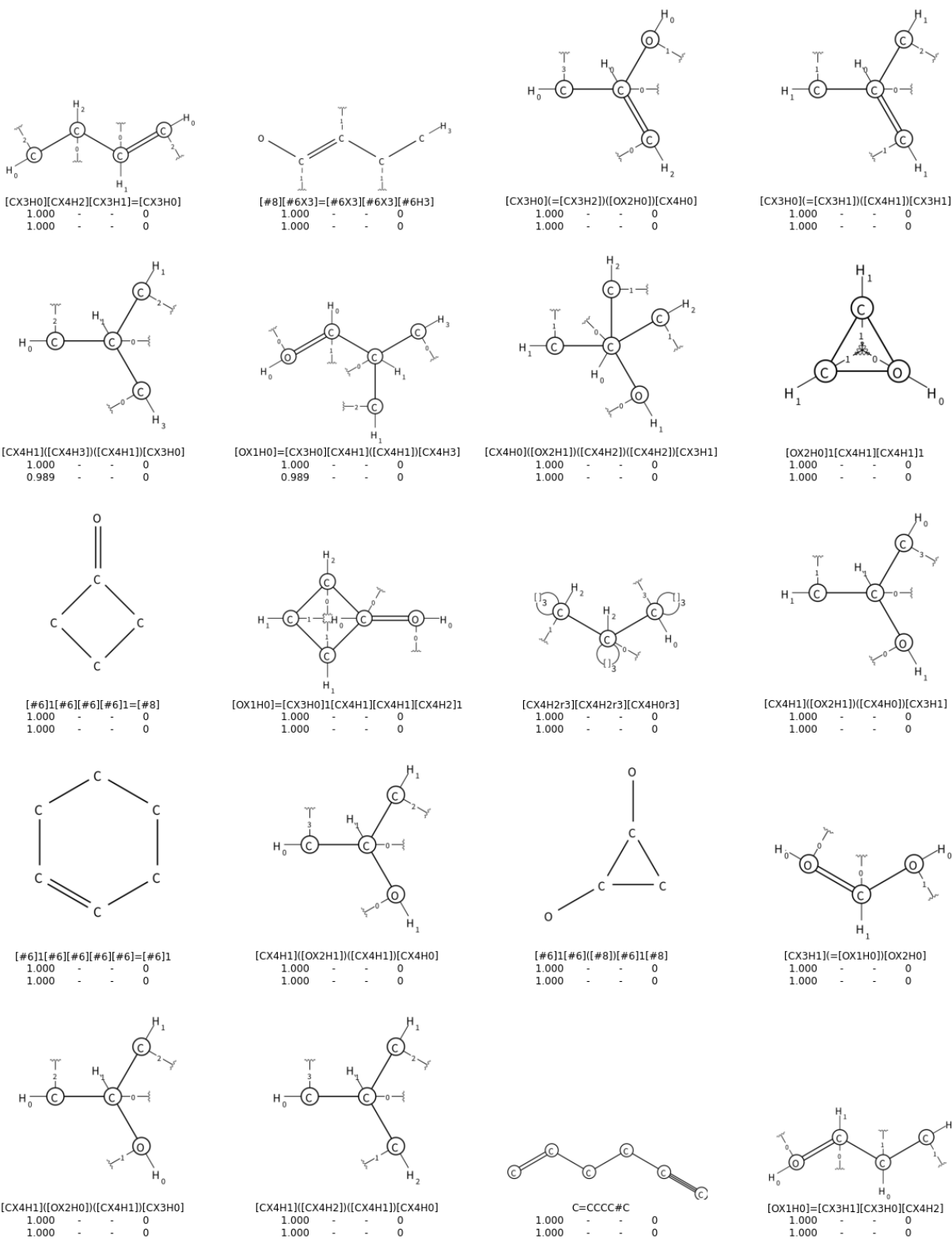


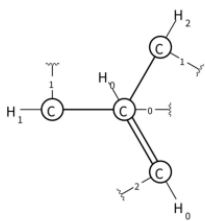
[OX2H0][CX4H1][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



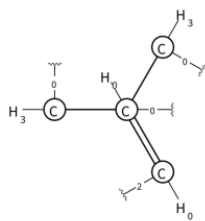
[CX4H0][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



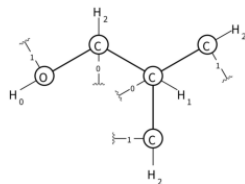




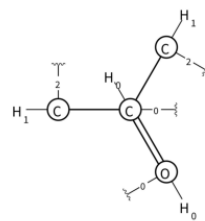
[CX3H0]=[CX3H0]([CX4H2])[CX3H1]
 1.000 - - 0
 1.000 - - 0



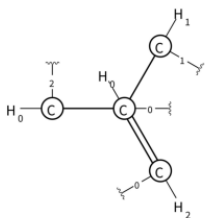
[CX3H0]=[CX3H0]([CX4H3])[CX4H3]
 1.000 - - 0
 1.000 - - 0



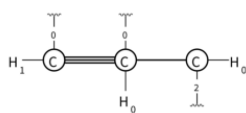
[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H2]
 1.000 - - 0
 1.000 - - 0



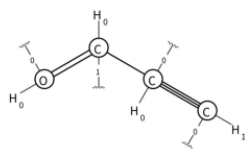
[CX3H0]=[OX1H0]([CX4H1])[CX4H1]
 1.000 - - 0
 1.000 - - 0



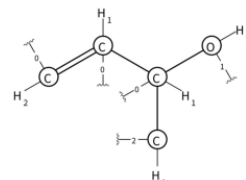
[CX3H0]=[CX3H2]([CX3H1])[CX3H0]
 1.000 - - 0
 1.000 - - 0



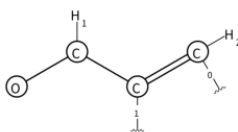
[CX2H0](#[CX2H1])[CX3H0]
 1.000 - - 0
 1.000 - - 0



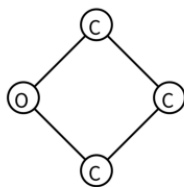
[OX1H0]=[CX3H0][CX2H0]#[CX2H1]
 1.000 - - 0
 1.000 - - 0



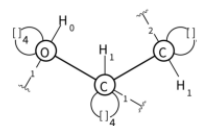
[CX3H2]=[CX3H1][CX4H1]([CX4H1])[OX2H0]
 1.000 - - 0
 1.000 - - 0



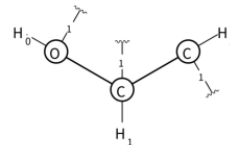
O[CH][CX3]=[CX3H2]
 1.000 - - 0
 1.000 - - 0



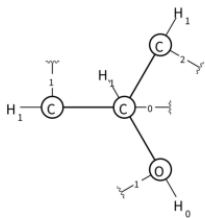
C1COC1
 1.000 - - 0
 1.000 - - 0



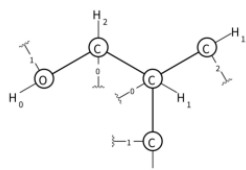
[OX2H0r4][CX4H1r4][CX4H1r4]
 1.000 - - 0
 1.000 - - 0



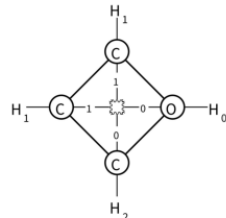
[OX2H0][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



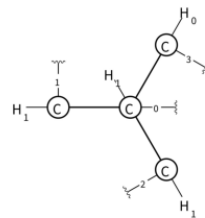
[CX4H1]([OX2H0])([CX4H1])[CX3H1]
 1.000 - - 0
 1.000 - - 0



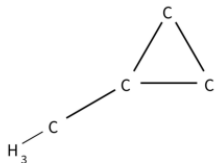
[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



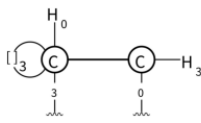
[OX2H0]1[CX4H2][CX4H1][CX4H1]1
 1.000 - - 0
 1.000 - - 0



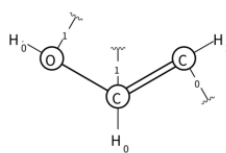
[CX4H1]([CX4H1])([CX4H0])[CX3H1]
 1.000 - - 0
 1.000 - - 0



#[6]1#[6]([#6H3])[#6]1
 1.000 - - 0
 1.000 - - 0



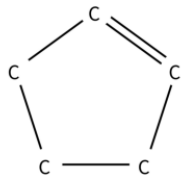
[CX4H3][CX4H0r3]
 1.000 - - 0
 1.000 - - 0



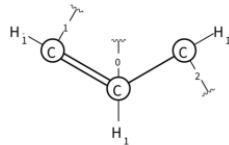
[OX2H0][CX3H0]=[CX3H2]
 1.000 - - 0
 0.989 - - 0



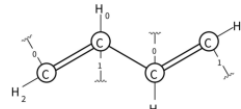
C=CCCC=C
 1.000 - - 0
 1.000 - - 0



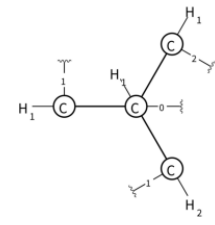
[#6]1[#6][#6][#6]=[#6]1
 1.000 - - 0
 1.000 - - 0



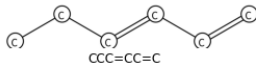
[CX3H1][=][CX3H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



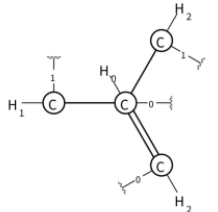
[CX3H2]=[CX3H0][CX3H1]=[CX3H1]
 1.000 - - 0
 1.000 - - 0



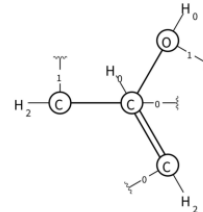
[CX4H1][CX4H2][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



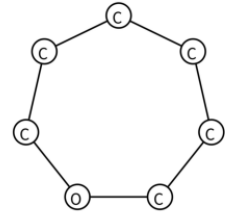
CCC=CC=C
 1.000 - - 0
 1.000 - - 0



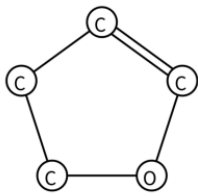
[CX3H0]=[CX3H2][CX4H2][CX3H1]
 1.000 - - 0
 1.000 - - 0



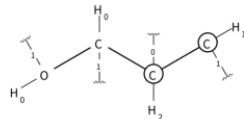
[CX3H0]=[CX3H2][OX2H0][CX4H2]
 1.000 - - 0
 1.000 - - 0



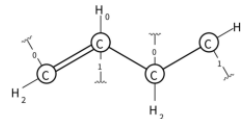
C1OCCCCC1
 1.000 - - 0
 1.000 - - 0



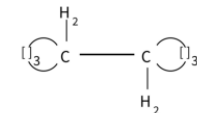
O1CCC=C1
 1.000 - - 0
 1.000 - - 0



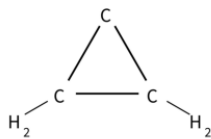
[#8X2H0][#6X3H0][CX4H2][CX3H1]
 1.000 - - 0
 1.000 - - 0



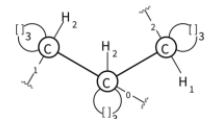
[CX3H2]=[CX3H0][CX4H2][CX3H1]
 1.000 - - 0
 1.000 - - 0



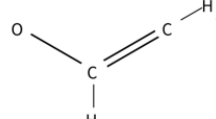
[#6H2r3][#6H2r3]
 1.000 - - 0
 1.000 - - 0



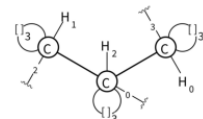
[#6H2]1[#6H2][#6]1
 1.000 - - 0
 1.000 - - 0



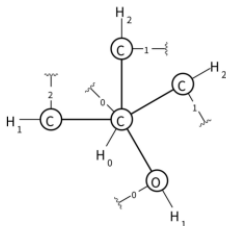
[CX4H2r3][CX4H2r3][CX4H1r3]
 1.000 - - 0
 1.000 - - 0



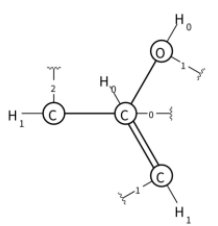
[#8][#6H0]=[#6H1]
 1.000 - - 0
 1.000 - - 0



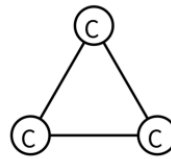
[CX4H1r3][CX4H2r3][CX4H0r3]
 1.000 - - 0
 1.000 - - 0



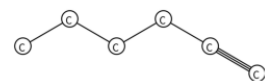
[CX4H0][OX2H1][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



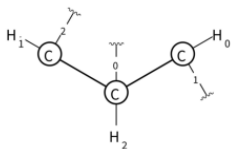
[CX3H0]=[CX3H1][OX2H0][CX4H1]
 1.000 - - 0
 1.000 - - 0



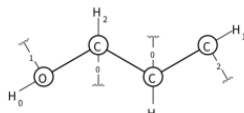
C1CC1
 1.000 - - 0
 1.000 - - 0



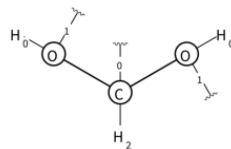
CCCC#C
 1.000 - - 0
 1.000 - - 0



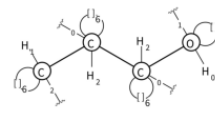
[CX4H2]([CX4H1])[CX2H0]
 1.000 - - 0
 1.000 - - 0



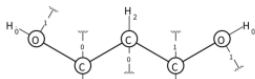
[OX2H0][CX4H2][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



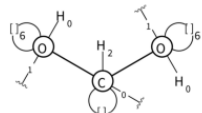
[CX4H2]([OX2H0])[OX2H0]
 1.000 - - 0
 1.000 - - 0



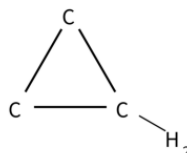
[CX4H1r6][CX4H2r6][CX4H2r6][OX2H0r6]
 1.000 - - 0
 1.000 - - 0



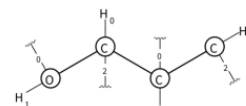
[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]
 1.000 - - 0
 1.000 - - 0



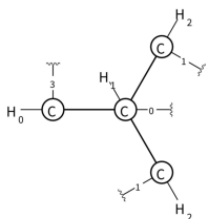
[OX2H0r6][CX4H2r6][OX2H0r6]
 1.000 - - 0
 1.000 - - 0



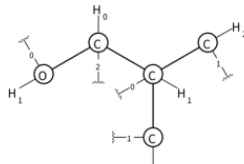
[#6H2]1[#6]1
 1.000 - - 0
 1.000 - - 0



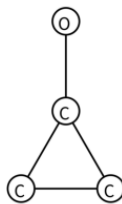
[OX2H1][CX4H0][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



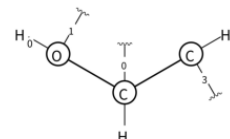
[CX4H1]([CX4H2])([CX4H2])[CX4H0]
 1.000 - - 0
 1.000 - - 0



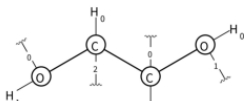
[OX2H1][CX4H0][CX4H1][CX4H2][CX4H2]
 1.000 - - 0
 1.000 - - 0



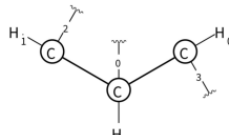
C1CC1O
 1.000 - - 0
 1.000 - - 0



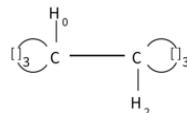
[CX4H2]([OX2H0])[CX4H0]
 1.000 - - 0
 1.000 - - 0



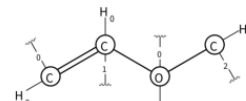
[OX2H1][CX4H0][CX4H2][OX2H0]
 1.000 - - 0
 1.000 - - 0



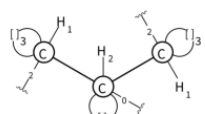
[CX4H2]([CX4H1])[CX4H0]
 1.000 - - 0
 1.000 - - 0



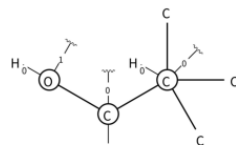
[#6H2r3][#6H0r3]
 1.000 - - 0
 1.000 - - 0



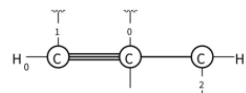
[CX3H2]=[CX3H0][OX2H0][CX3H0]
 1.000 - - 0
 1.000 - - 0



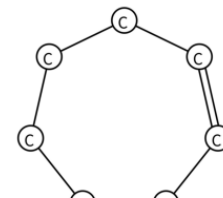
[CX4H1r3][CX4H2r3][CX4H1r3]
 1.000 - - 0
 1.000 - - 0



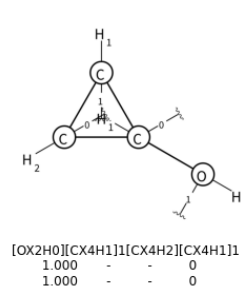
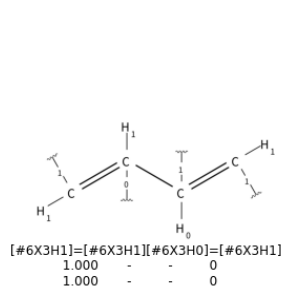
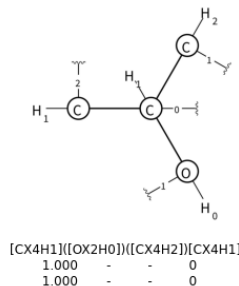
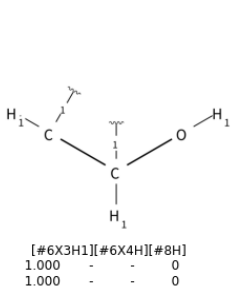
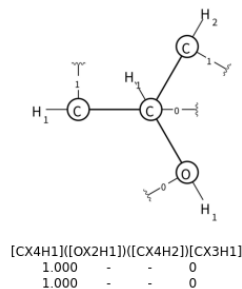
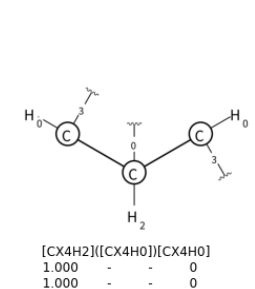
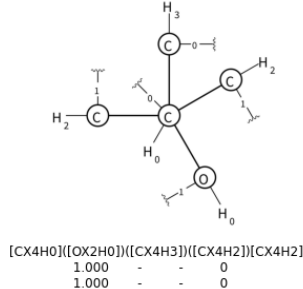
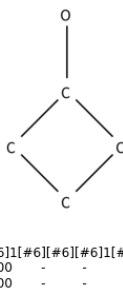
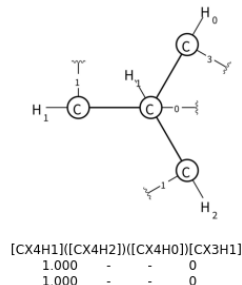
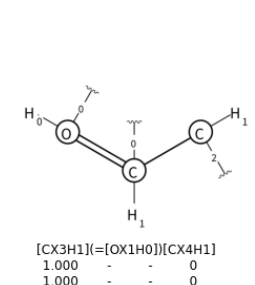
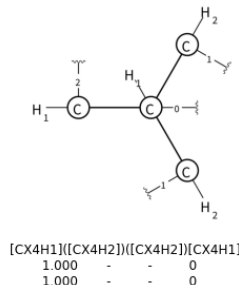
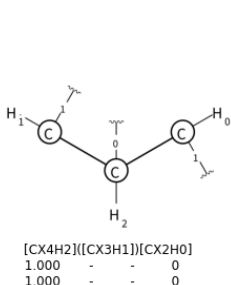
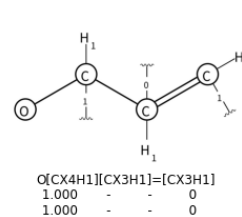
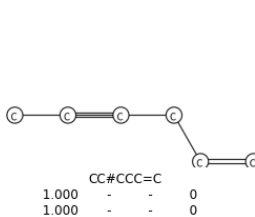
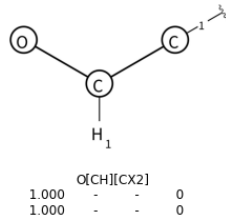
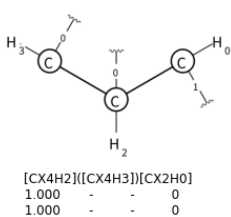
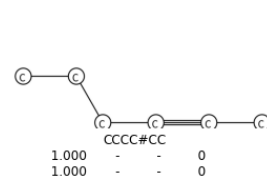
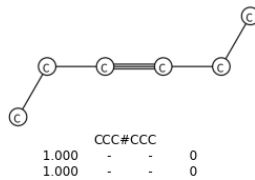
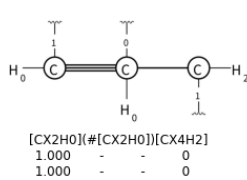
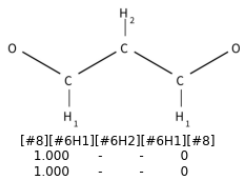
[OX2H0][CX4H2][CX4H0]([#6])([#6])([#6])
 1.000 - - 0
 1.000 - - 0

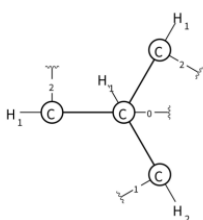


[CX2H0]([#CX2H0])[CX4H1]
 1.000 - - 0
 1.000 - - 0

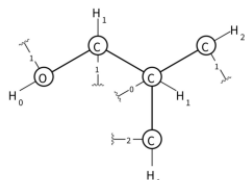


C1OCCCC=C1
 1.000 - - 0
 1.000 - - 0

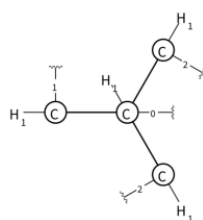




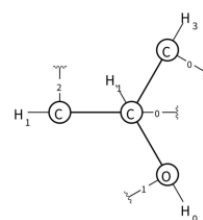
[CX4H1][CX4H2][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



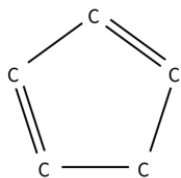
[OX2H0][CX4H1][CX4H1][CX4H1][CX4H2]
 1.000 - - 0
 1.000 - - 0



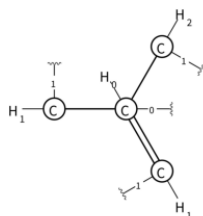
[CX4H1][CX4H1][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



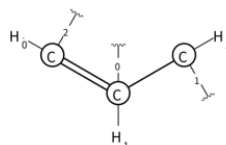
[CX4H1][OX2H0][CX4H3][CX4H1]
 1.000 - - 0
 1.000 - - 0



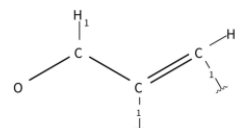
[#6][#6][#6][#6][#6]1
 1.000 - - 0
 1.000 - - 0



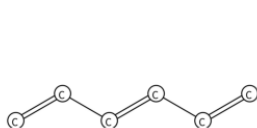
[CX3H0]=[CX3H1][CX4H2][CX3H1]
 1.000 - - 0
 1.000 - - 0



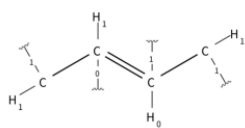
[CX3H1]=[CX3H0][CX3H1]
 1.000 - - 0
 1.000 - - 0



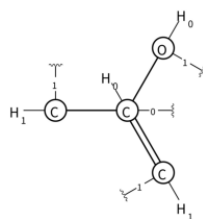
[#8][#6H][#6X3][#6X3H]
 1.000 - - 0
 1.000 - - 0



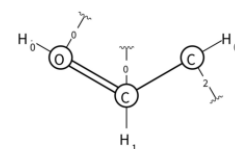
C=CC=CC
 1.000 - - 0
 1.000 - - 0



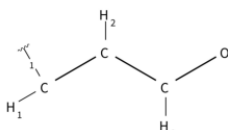
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]
 1.000 - - 0
 1.000 - - 0



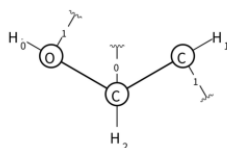
[CX3H0]=[CX3H1][OX2H0][CX3H1]
 1.000 - - 0
 1.000 - - 0



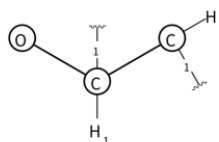
[CX3H1]=[OX1H0][CX3H0]
 1.000 - - 0
 1.000 - - 0



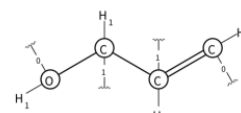
[#6X3H][#6H2][#6H2][#8]
 1.000 - - 0
 1.000 - - 0



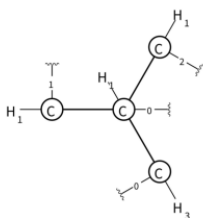
[CX4H2][OX2H0][CX3H1]
 1.000 - - 0
 1.000 - - 0



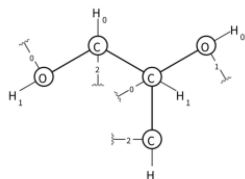
O[CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



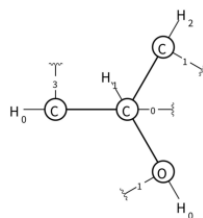
[OX2H1][CX4H1][CX3H0]=[CX3H2]
 1.000 - - 0
 1.000 - - 0



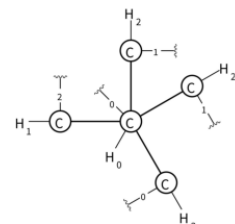
[CX4H1][CX4H3][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



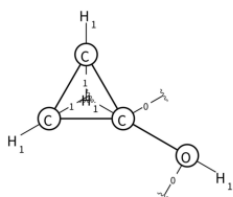
[OX2H1][CX4H0][CX4H1][CX4H1][OX2H0]
 1.000 - - 0
 1.000 - - 0



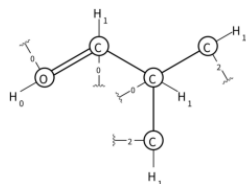
[CX4H1][OX2H0][CX4H2][CX4H0]
 1.000 - - 0
 1.000 - - 0



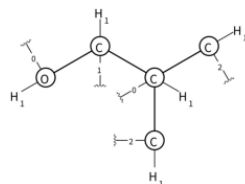
[CX4H0][CX4H3][CX4H2][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



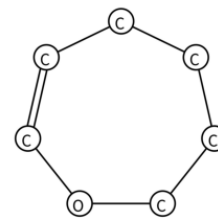
[OX2H1][CX4H1]1[CX4H1][CX4H1]1
 1.000 - - 0
 1.000 - - 0



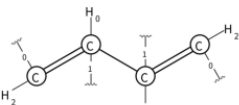
[OX1H0]=[CX3H1][CX4H1]1[CX4H1]1[CX4H1]1
 1.000 - - 0
 1.000 - - 0



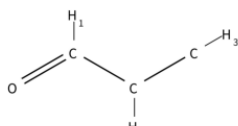
[OX2H1][CX4H1]1[CX4H1]1[CX4H1]1[CX4H1]1
 1.000 - - 0
 1.000 - - 0



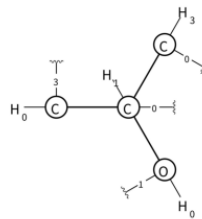
C1OC=CCCC1
 1.000 - - 0
 1.000 - - 0



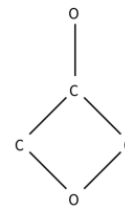
[CX3H2]=[CX3H0][CX3H0]=[CX3H2]
 1.000 - - 0
 1.000 - - 0



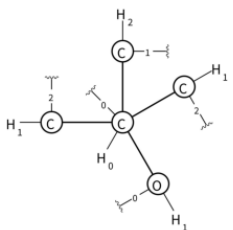
[#8]=[#6H1][#6H1][#6H3]
 1.000 - - 0
 1.000 - - 0



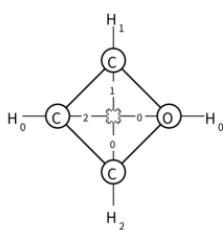
[CX4H1]1([OX2H0])([CX4H3])[CX4H0]
 1.000 - - 0
 1.000 - - 0



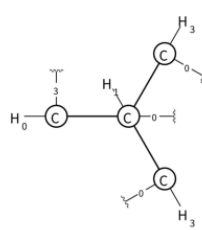
[#6]1[#8][#6][#6]1[#8]
 1.000 - - 0
 1.000 - - 0



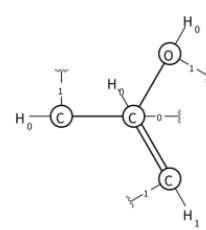
[CX4H0]1([OX2H1])([CX4H2])([CX4H1])[CX4H1]
 1.000 - - 0
 1.000 - - 0



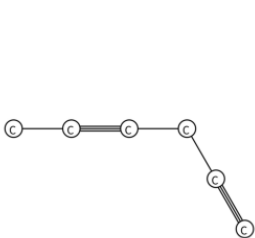
[OX2H0]1[CX4H2][CX4H0][CX4H1]1
 1.000 - - 0
 1.000 - - 0



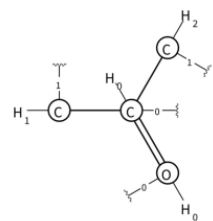
[CX4H1]1([CX4H3])([CX4H3])[CX4H0]
 1.000 - - 0
 1.000 - - 0



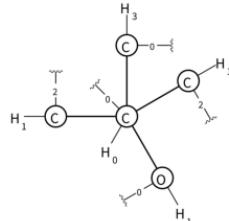
[CX3H0]=[CX3H1]1([OX2H0])[CX2H0]
 1.000 - - 0
 1.000 - - 0



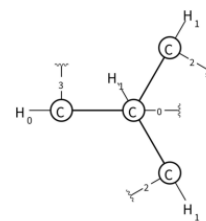
CC#CCC#C
 1.000 - - 0
 1.000 - - 0



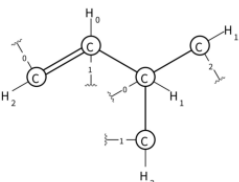
[CX3H0]=[OX1H0]1([CX4H2])[CX3H1]
 1.000 - - 0
 1.000 - - 0



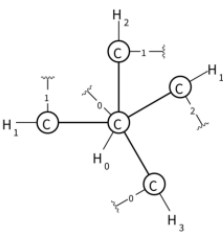
[CX4H0]1([OX2H1])([CX4H3])([CX4H1])[CX4H1]
 1.000 - - 0
 1.000 - - 0



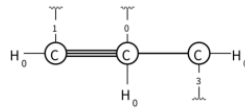
[CX4H1]1([CX4H1])([CX4H1])[CX4H0]
 1.000 - - 0
 1.000 - - 0



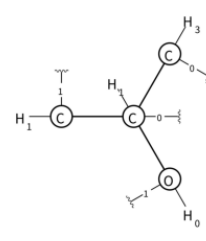
[CX3H2]=[CX3H0][CX4H1]1([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



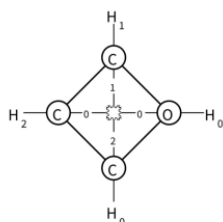
[CX4H0]1([CX4H3])([CX4H2])([CX4H1])[CX3H1]
 1.000 - - 0
 1.000 - - 0



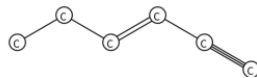
[CX2H0]1([#][CX2H0])[CX4H0]
 1.000 - - 0
 1.000 - - 0



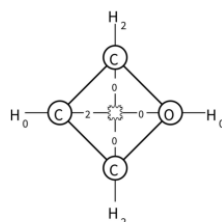
[CX4H1]1([OX2H0])([CX4H3])[CX3H1]
 1.000 - - 0
 1.000 - - 0



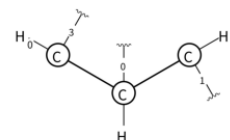
[OX2H0][CX4H0][CX4H2][CX4H1]1
 1.000 - - 0
 1.000 - - 0



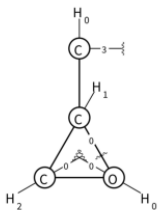
CCC=CC#C
 1.000 - - 0
 1.000 - - 0



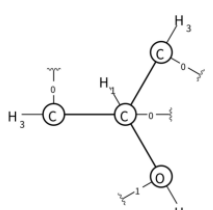
[OX2H0]1[CX4H2][CX4H0][CX4H2]1
 1.000 - - 0
 1.000 - - 0



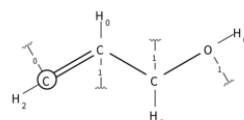
[CX4H2][CX4H0][CX2H0]
 1.000 - - 0
 1.000 - - 0



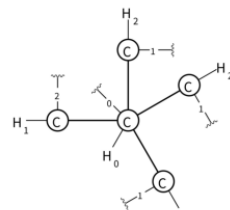
[OX2H0][CX4H2][CX4H1]1[CX4H0]
 1.000 - - 0
 1.000 - - 0



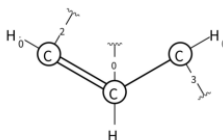
[CX4H1][OX2H0][CX4H3][CX4H3]
 1.000 - - 0
 1.000 - - 0



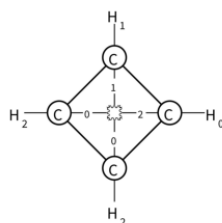
[CX3H2]=[#6X3H0][#6X3H0][#8X2H0]
 1.000 - - 0
 1.000 - - 0



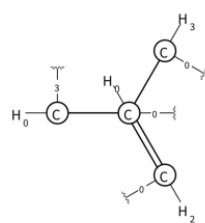
[CX4H0][CX4H2][CX4H2][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



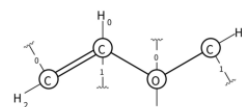
[CX3H1]=[CX3H0][CX4H0]
 1.000 - - 0
 1.000 - - 0



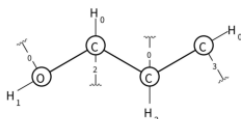
[CX4H0][CX4H2][CX4H2][CX4H1]1
 1.000 - - 0
 1.000 - - 0



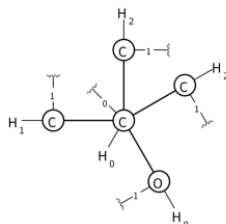
[CX3H0]=[CX3H2][CX4H3][CX4H0]
 1.000 - - 0
 1.000 - - 0



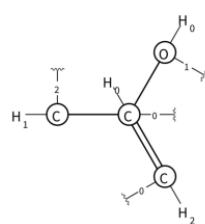
[CX3H2]=[CX3H0][OX2H0][CX4H2]
 1.000 - - 0
 1.000 - - 0



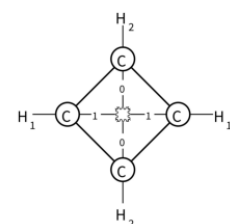
[OX2H1][CX4H0][CX4H2][CX4H0]
 1.000 - - 0
 1.000 - - 0



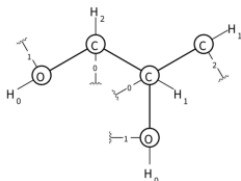
[CX4H0][OX2H0][CX4H2][CX4H2][CX3H1]
 1.000 - - 0
 1.000 - - 0



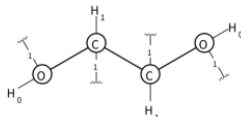
[CX3H0]=[CX3H2][OX2H0][CX4H1]
 1.000 - - 0
 1.000 - - 0



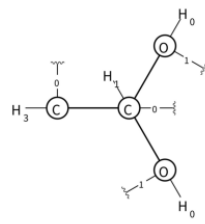
[CX4H1][CX4H2][CX4H1][CX4H2]1
 1.000 - - 0
 1.000 - - 0



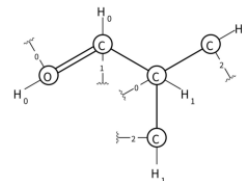
[OX2H0][CX4H2][CX4H1][OX2H0][CX4H1]
 1.000 - - 0
 1.000 - - 0



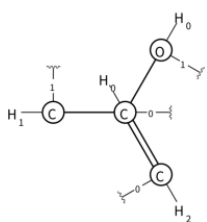
[OX2H0][CX4H1][CX4H1][OX2H0]
 1.000 - - 0
 1.000 - - 0



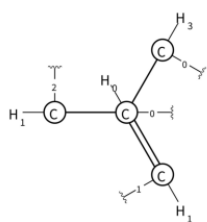
[CX4H1][OX2H0][OX2H0][CX4H3]
 1.000 - - 0
 1.000 - - 0



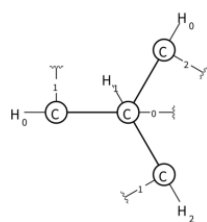
[OX1H0]=[CX3H0][CX4H1][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



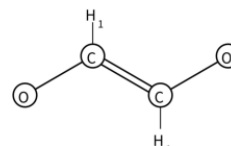
[CX3H0](=[CX3H2])[(OX2H0)](CX3H1)
 1.000 - - 0
 1.000 - - 0



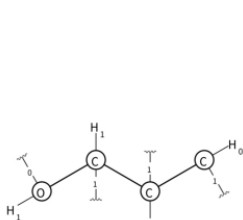
[CX3H0](=[CX3H1])[(CX4H3)](CX4H1)
 1.000 - - 0
 1.000 - - 0



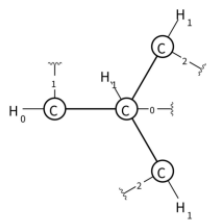
[CX4H1]((CX4H2))((CX3H0))(CX2H0)
 1.000 - - 0
 1.000 - - 0



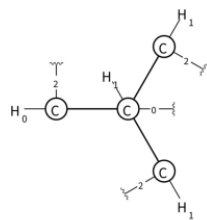
O(CH)=[CH]O
 1.000 - - 0
 1.000 - - 0



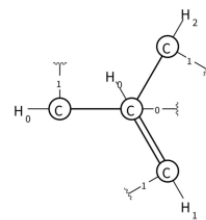
[OX2H1][CX4H1][CX4H1][CX2H0]
 1.000 - - 0
 1.000 - - 0



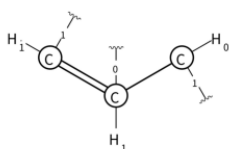
[CX4H1]((CX4H1))((CX4H1))(CX2H0)
 1.000 - - 0
 1.000 - - 0



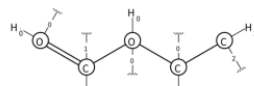
[CX4H1]((CX4H1))((CX4H1))(CX3H0)
 1.000 - - 0
 1.000 - - 0



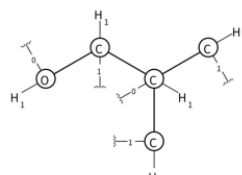
[CX3H0](=[CX3H1])[(CX4H2)](CX2H0)
 1.000 - - 0
 1.000 - - 0



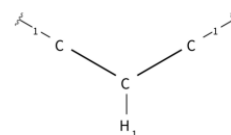
[CX3H1](=[CX3H1])(CX2H0)
 1.000 - - 0
 1.000 - - 0



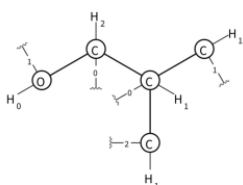
[OX1H0](=[CX3H0])(OX2H0)[CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



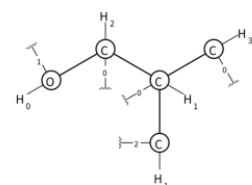
[OX2H1][CX4H1][CX4H1]((CX4H2))(CX4H2)
 1.000 - - 0
 1.000 - - 0



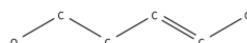
[#6X2][#6H1][#6X2]
 1.000 - - 0
 1.000 - - 0



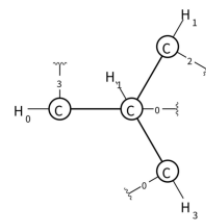
[OX2H0][CX4H2][CX4H1]((CX4H1))(CX3H1)
 1.000 - - 0
 1.000 - - 0



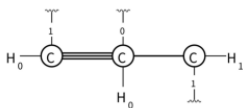
[OX2H0][CX4H2][CX4H1]((CX4H1))(CX4H3)
 1.000 - - 0
 1.000 - - 0



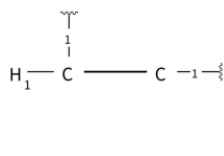
[#8][#6][#6][#6][#6][#8]
 1.000 - - 0
 1.000 - - 0



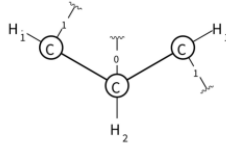
[CX4H1]((CX4H3))((CX4H1))(CX4H0)
 1.000 - - 0
 1.000 - - 0



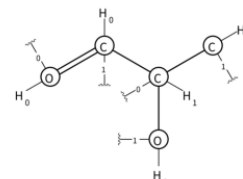
[CX2H0](#[CX2H0])(CX3H1)
 1.000 - - 0
 1.000 - - 0



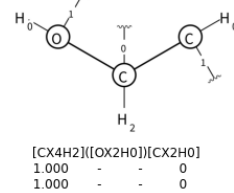
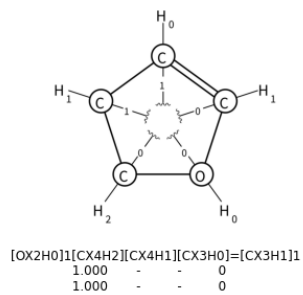
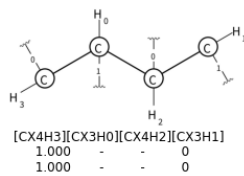
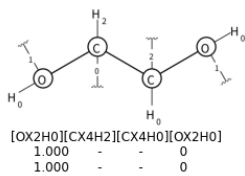
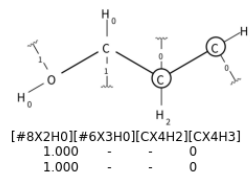
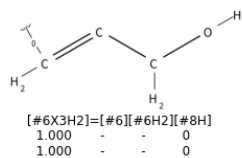
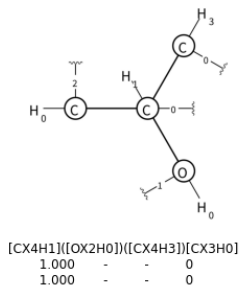
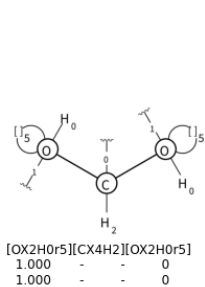
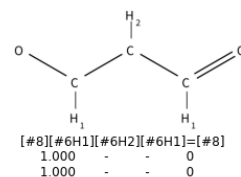
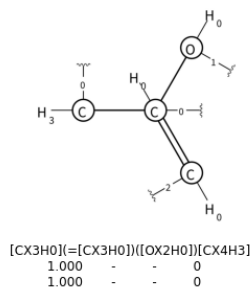
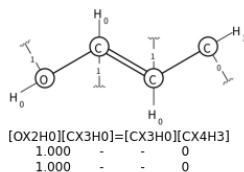
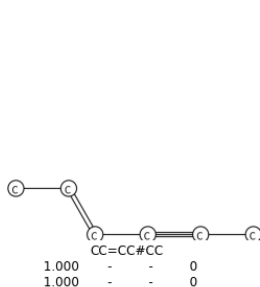
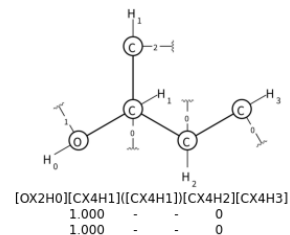
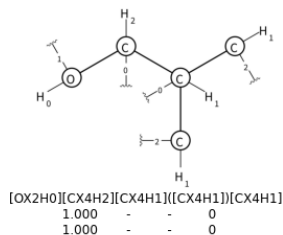
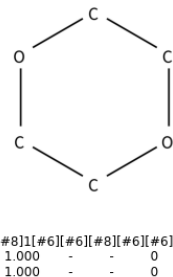
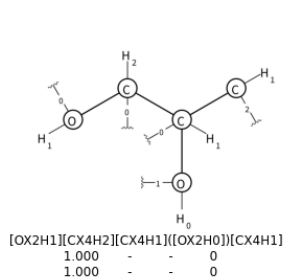
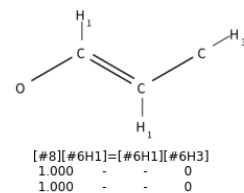
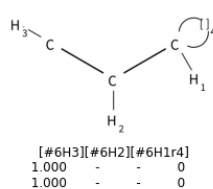
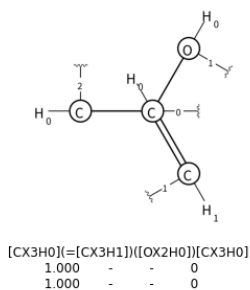
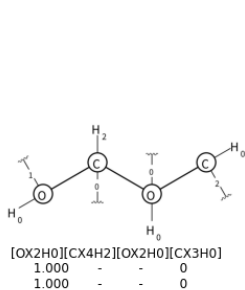
[#6X2][#6X3H]
 1.000 - - 0
 1.000 - - 0

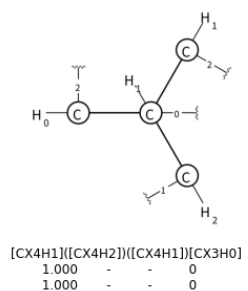
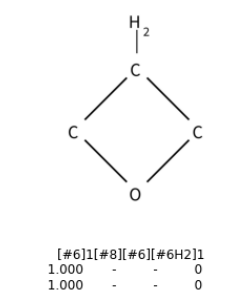
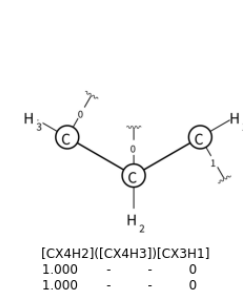
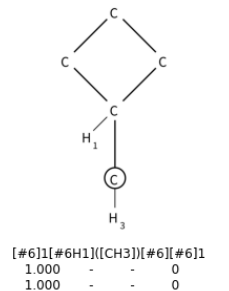
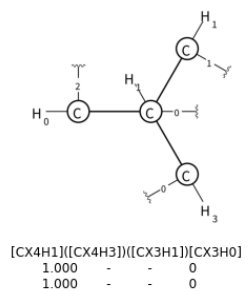
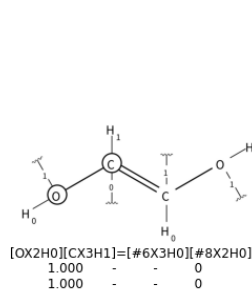
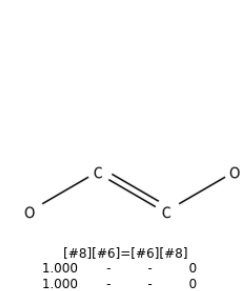
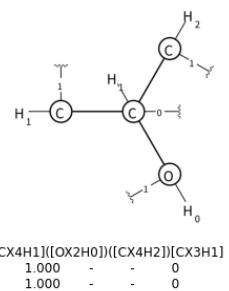
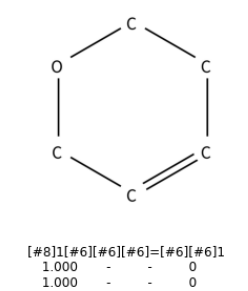
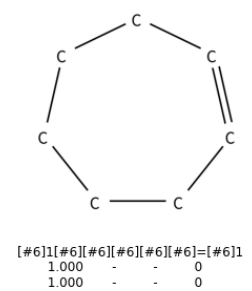
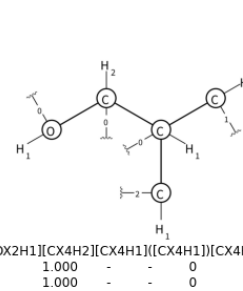
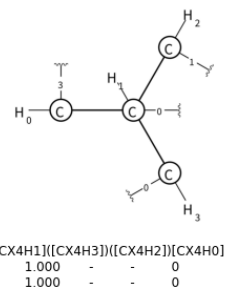
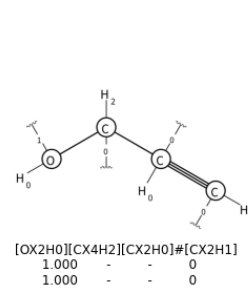
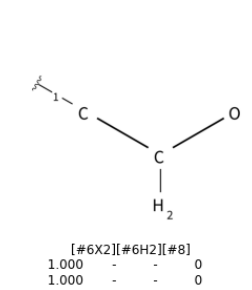
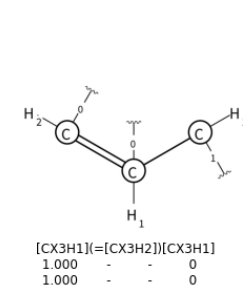
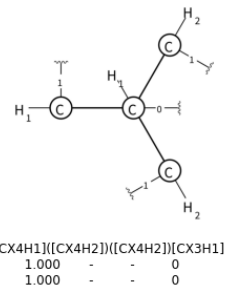
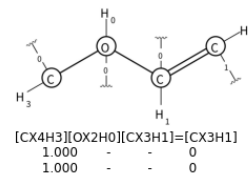
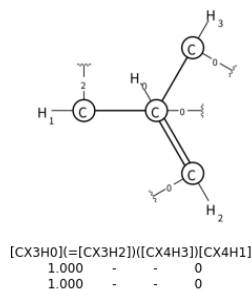
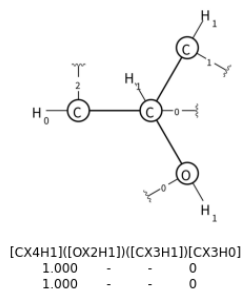
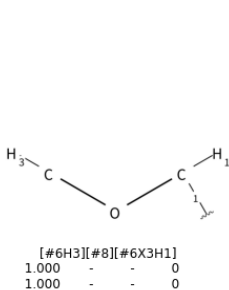


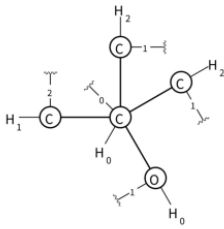
[CX4H2]((CX3H1))(CX3H1)
 1.000 - - 0
 1.000 - - 0



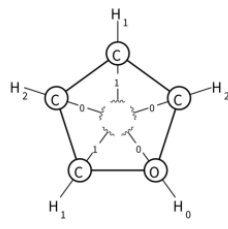
[OX1H0](CX3H0)[CX4H1]((OX2H0))(CX4H2)
 1.000 - - 0
 1.000 - - 0



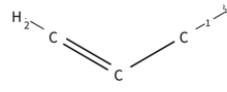




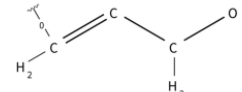
[CX4H0]([OX2H0])([CX4H2])([CX4H2])[CX4H1]
 1.000 - - 0
 1.000 - - 0



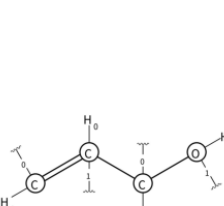
[OX2H0]1[CX4H1][CX4H2][CX4H1][CX4H2]1
 1.000 - - 0
 1.000 - - 0



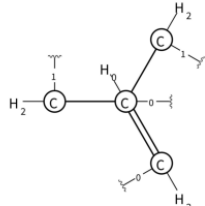
[#6H2]=[#6][#6X2]
 1.000 - - 0
 1.000 - - 0



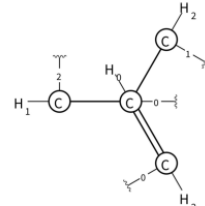
[#6X3H2]=[#6][#6H2][#8]
 1.000 - - 0
 1.000 - - 0



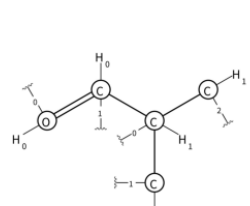
[CX3H2]=[CX3H0][CX4H2][OX2H0]
 1.000 - - 0
 1.000 - - 0



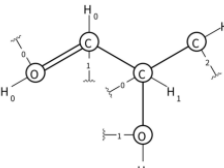
[CX3H0]=[CX3H2][CX4H2][CX4H2]
 1.000 - - 0
 1.000 - - 0



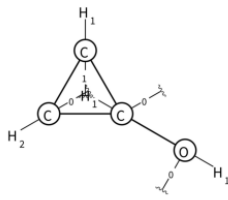
[CX3H0]=[CX3H2][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



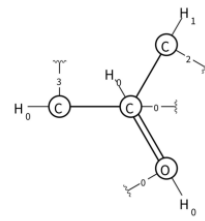
[OX1H0]=[CX3H0][CX4H1][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



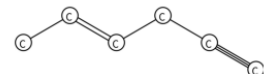
[OX1H0]=[CX3H0][CX4H1][OX2H0][CX4H1]
 1.000 - - 0
 1.000 - - 0



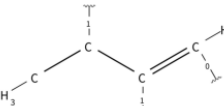
[OX2H1][CX4H1]1[CX4H2][CX4H1]1
 1.000 - - 0
 1.000 - - 0



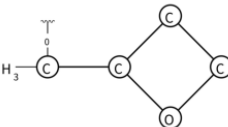
[CX3H0]=[OX1H0][CX4H1][CX4H0]
 1.000 - - 0
 1.000 - - 0



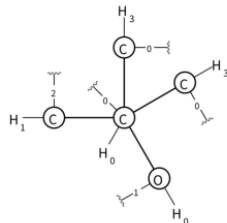
CC=CCC#C
 1.000 - - 0
 1.000 - - 0



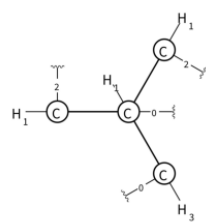
[#6H3][#6X3][#6X3]=[#6X3H2]
 1.000 - - 0
 1.000 - - 0



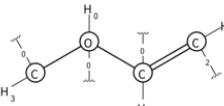
C1OC([CX4H3])C1
 1.000 - - 0
 1.000 - - 0



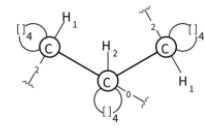
[CX4H0]([OX2H0])([CX4H3])([CX4H3])[CX4H1]
 1.000 - - 0
 1.000 - - 0



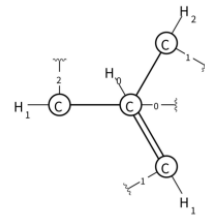
[CX4H1][CX4H3][CX4H1][CX4H1]
 1.000 - - 0
 1.000 - - 0



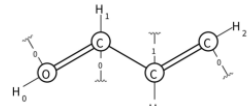
[CX4H3][OX2H0][CX3H1]=[CX3H0]
 1.000 - - 0
 1.000 - - 0



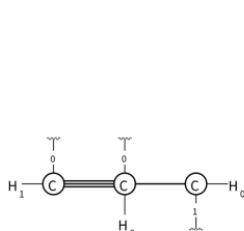
[CX4H1r4][CX4H2r4][CX4H1r4]
 1.000 - - 0
 1.000 - - 0



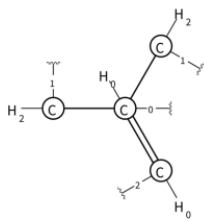
[CX3H0]=[CX3H1][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



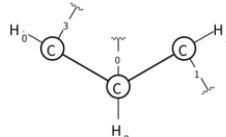
[OX1H0]=[CX3H1][CX3H0]=[CX3H2]
 1.000 - - 0
 1.000 - - 0



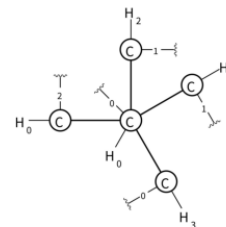
[CX2H0][#CX2H1][CX2H0]
 1.000 - - 0
 1.000 - - 0



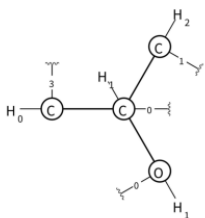
[CX3H0]=[CX3H0][CX4H2][CX4H2]
 1.000 - - 0
 1.000 - - 0



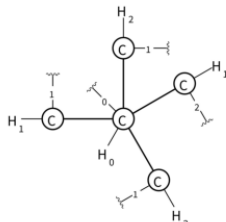
[CX4H2][CX4H0][CX3H1]
 1.000 - - 0
 1.000 - - 0



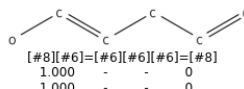
[CX4H0][CX4H3][CX4H2][CX4H2][CX3H0]
 1.000 - - 0
 1.000 - - 0



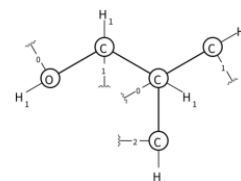
[CX4H1][OX2H1][CX4H2][CX4H0]
 1.000 - - 0
 1.000 - - 0



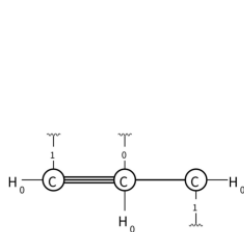
[CX4H0][CX4H2][CX4H2][CX4H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



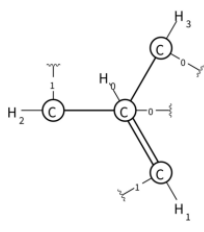
[#8][#6]=[#6][#6]=[#6]
 1.000 - - 0
 1.000 - - 0



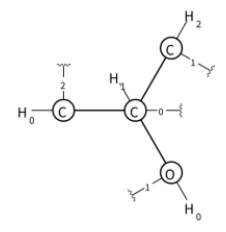
[OX2H1][CX4H1][CX4H1][CX4H1][CX4H2]
 1.000 - - 0
 1.000 - - 0



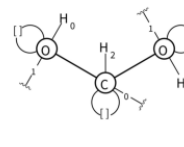
[CX2H0][#CX2H0][CX2H0]
 1.000 - - 0
 1.000 - - 0



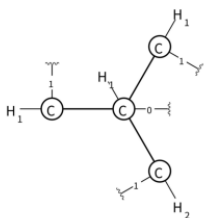
[CX3H0]=[CX3H1][CX4H3][CX4H2]
 1.000 - - 0
 1.000 - - 0



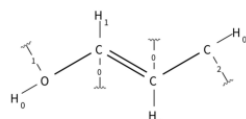
[CX4H1][OX2H0][CX4H2][CX3H0]
 1.000 - - 0
 1.000 - - 0



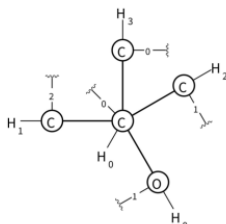
[OX2H0r0][CX4H2r0][OX2H0r0]
 1.000 - - 0
 1.000 - - 0



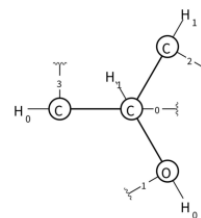
[CX4H1][CX4H2][CX3H1][CX3H1]
 1.000 - - 0
 1.000 - - 0



[#8X2H0][#6X3H1]=[#6X3H1][#6X3H0]
 1.000 - - 0
 1.000 - - 0



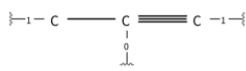
[CX4H0][OX2H0][CX4H3][CX4H2][CX4H1]
 1.000 - - 0
 1.000 - - 0



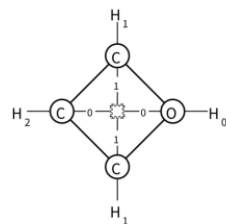
[CX4H1][OX2H0][CX4H1][CX4H0]
 1.000 - - 0
 1.000 - - 0



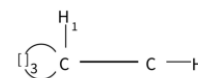
CCC#CC#C
 1.000 - - 0
 1.000 - - 0



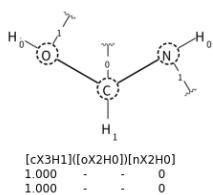
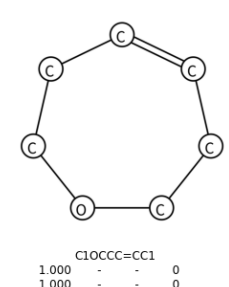
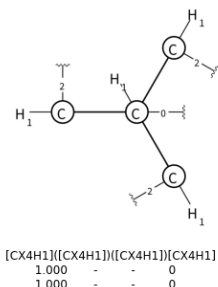
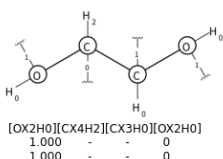
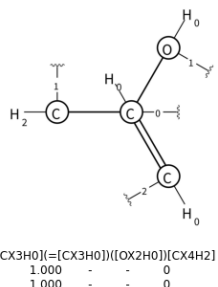
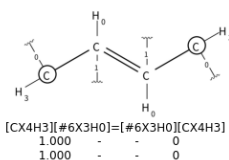
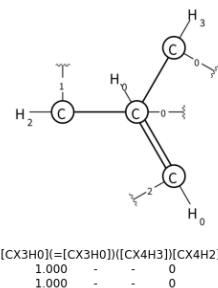
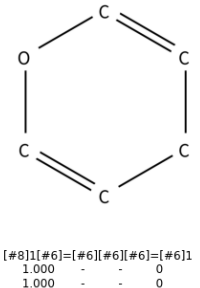
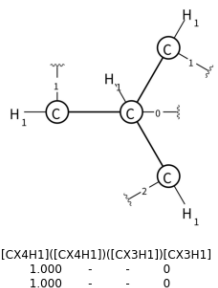
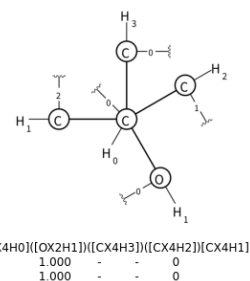
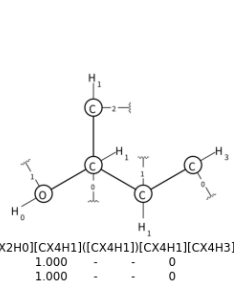
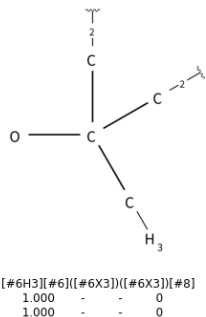
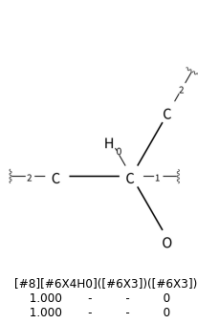
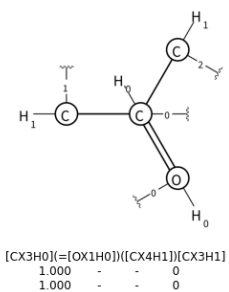
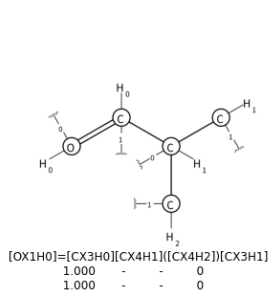
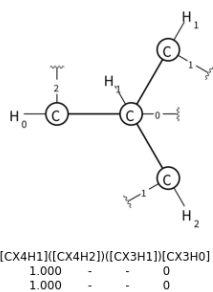
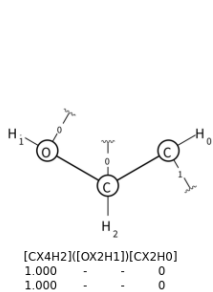
[#6X2][#6X2][#6X2]
 1.000 - - 0
 1.000 - - 0



[OX2H0]1[CX4H1][CX4H2][CX4H1]1
 1.000 - - 0
 1.000 - - 0



[#6H3][#6H1r3]
 1.000 - - 0
 1.000 - - 0



4.3 Validation dataset results

See validation_results.pdf

Sorted by number of possible structures. Index of -1 indicates that the correct structure was not generated. Number of total possible structures is calculated from the number of structures generated using OMG after filtering with the list of unstable or unlikely substructures.

4.4 Test dataset results

See test_results.pdf

Sorted by number of possible structures. Index of -1 indicates that the correct structure was not generated. Number of total possible structures is calculated from the number of structures generated using OMG after filtering with the list of unstable or unlikely substructures.

See largermolecule_test_results.pdf for the substructure results of the set of 8 larger molecules containing between 12 and 14 non-hydrogen atoms.

4.5 Annotation results

Annotation of picked ^1H and ^{13}C peaks in selected test examples.

See test_annotation_results.pdf

5 References

1. Landrum, G. RDKit: Open-source cheminformatics.
2. Weininger, D. SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules. *J. Chem. Inf. Model.* **28**, 31–36 (1988).
3. Wunderlich, R. E., Wenisch, T. F., Falsafi, B. & Hoe, J. C. SMARTS. in *Proceedings of the 30th annual international symposium on Computer architecture - ISCA '03 84* (ACM Press, 2003). doi:10.1145/859618.859629
4. Blum, L. C. & Reymond, J. L. 970 Million druglike small molecules for virtual screening in the chemical universe database GDB-13. *J. Am. Chem. Soc.* **131**, 8732–8733 (2009).
5. O'Boyle, N. M. *et al.* Open Babel: An Open chemical toolbox. *J. Cheminform.* **3**, 1–14 (2011).
6. Mestrelab Research S.L. MestReNova. (2020).
7. Wishart, D. S. *et al.* HMDB 4.0: The human metabolome database for 2018. *Nucleic Acids Res.* **46**, D608–D617 (2018).
8. SDBSWeb : <https://sdb.sdb.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, 2021)
9. Khan, A., Sohail, A., Zahoora, U. & Qureshi, A. S. A survey of the recent architectures of deep convolutional neural networks. *Artif. Intell. Rev.* **53**, 5455–5516 (2020).
10. Peironcely, J. E. *et al.* OMG: Open molecule generator. *J. Cheminform.* **4**, 1–13 (2012).