Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Quantum-Mechanical Transition-State Model Combined with Machine Learning Provides Catalyst Design Features for Selective Cr Olefin Oligomerization

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Further Computational Details

All calculations were performed in Gaussian 09 revision B.01. Geometry optimizations were performed at the UM06L/6-31G(d,p) [LANL2DZ for Cr] level of theory. Vibrational frequencies were computed to verify stationary points as first-order saddle points (transition states). As mentioned in the main text, the M06L functional was used because it has been shown to be accurate for estimating reaction energies of first-row transition metal complexes. Solvent effects were modelled using the SMD solvation model for cyclohexane. Optimized electronic energies were further refined with single point calculations using the def2-TZVPP basis set. Final free energies reported are computed at the UM06L/Def2-TZVPP//UM06L/6-31G(d,p) [LANL2DZ] level of theory. Free energies are the sum of $E_{(Large)} + \Delta E_{ZPE(small)} + \Delta U_{vib(small)} + \Delta U_{rot(small)} + \Delta U_{trans(small)} + nRT - T\Delta S_{vib(small)} - T\Delta S_{rot(small)} - T\Delta S_{trans(small)} + \Delta G_{solv(large)}$. E if the total SCF energy. $\Delta E_{ZPE(small)}$ is the zero-point energy correction. $\Delta U_{vib(small)}$, $\Delta U_{rot(small)}$ and $\Delta U_{trans(small)}$ are thermal energy vibrational, rotational and translation corrections. R is the gas constant and T is the temperature (298.15K). $T\Delta S_{vib(small)}$, $T\Delta S_{rot(small)}$ and $T\Delta S_{trans(small)}$ are temperature dependent vibrational, rotational and translation entropy corrections. $\Delta G_{solv(large)}$ is the standard state solvation free energy change. Large = UM06L/Def2TZVPP. Small = UM06L/6-31G(d,p) [LANL2DZ for Cr].

Full G09 Reference: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision B.01. Wallingford CT, 2009.

Details of Machine Learning Analysis

The chosen machine learning regression algorithms (Random Forest, Gaussian Process Regression, LASSO, Elastic-Net, Support Vector Regression (radial basis function kernel), Support Vector Regression (linear kernel) were tentatively fit to our dataset in order to determine which method best modeled the trends in our data (see "Initial_Regression_Models" Jupyter notebook). A function was defined in order to compute the accuracy of each model and perform cross-validation. The average accuracy of a regression algorithm is determined by randomly sampling the datasets and performing cross-validation during each random sampling. In our study 10 random samples were taken and 20-fold cross-validation was performed at each validation. The data is randomly sampled 10 times to create 10 subsets of data, and each of these subsets would be divided into 20 partitions. An accuracy for the regressor was computed once with each of these 20 partitions as the test data, and the other 19 as training data. Overall, 200 accuracies are computed and then averaged. This procedure was adapted from a recent study by our group (*J. Phys. Chem. A* 2020, 124, 23, 4813–4826, doi: 10.1021/acs.jpca.9b10410).

As further validation of our method, Table S1 below provides the root mean square error (RMSE) computed with different numbers of random sampling and cross-validation. The amount of cross validation steps has a more significant impact on the RMSE than the number of random samplings of the dataset. The results presented in the main manuscript were obtained using 10 random samples with 20-fold cross-validation (200 total accuracies). This accuracy is significantly greater than that obtained by computing 20, 30, 100, or 150 accuracies, but indistinguishable from the RMSE computed using 300 accuracies.

Table S1. Root mean square errors of regression algorithms computed using different random sampling and cross-validation options.

	10x Random Sampling			15x Random Sampling		
# Cross Val.	2	10	20	2	10	20
Random Forest	0.886	0.426	0.344	0.886	0.422	0.345
LASSO	1.040	0.613	0.565	1.040	0.613	0.565
Elastic-Net	1.020	0.616	0.568	1.020	0.616	0.568
GPR	0.727	0.474	0.422	0.727	0.474	0.422
SVR-Linear	1.103	0.558	0.491	1.103	0.558	0.491
SVR-RBF	1.023	0.639	0.408	1.023	0.639	0.558
Ridge	1.140	0.565	0.494	1.140	0.565	0.494

Following the identification of random forest as the best regression model it was optimized by searching for the combination of hyperparameters that minimized the RMSE. The number of estimators (number of trees in the forest), maximum depth (number of splits of each tree), and maximum features (number of features considered at each split) were varied (see "Hyperparameter_Optimization_RF" Jupyter notebook for additional details). The RMSE for each combination of hyperparameters was computed using the random sampling and cross-validation method outlined above. Using the optimized RF model, the 1-hexene/1-octene selectivity of each ligand was computed (see "Selectivity_Predictions_RF" Jupyter notebook).

In order to determine the feature importance (see "RF_Feature_Importances" Jupyter notebook) by using 10 random samplings of the dataset with 20 iterations (total 200). The random forest model is fit to the dataset for each iteration and the feature importance, as determined from the sci-kit learn package and averaged. The final averaged feature importance along with the 95% confidence interval is printed.

The source code is provided below, and further details and documentation is provided in the Jupyter notebooks in the supporting information.

Source Code

Initial Regression Model Testing

```
# Import needed packages

import numpy as np
import pandas as pd
import pandas_profiling
import scipy.stats
from sklearn.neural_network import MLPRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.svm import SVR
from sklearn import linear_model
from sklearn.linear_model import Ridge, Lasso, ElasticNet
from sklearn.model_selection import cross_val_score
import seaborn as sns

#Read in data and remove non-essential columns
data = pd.read_csv("dataset.csv")
data = data.drop("Catalyst", axis = 1)


#Make dataframe to record accuracy of models
Accuracy_df = pd.DataFrame(columns =['Model', 'Accuracy'])


#Compute 95% Confidence Interval
def mean_confidence_interval(data, confidence=0.95):
   a = 1.0 * np.array(data)
   n = len(a)
   m, se = np.mean(a), scipy.stats.sem(a)
   h = se * scipy.stats.t.ppf((1 + confidence) / 2., n-1)
   return m, m-h, m+h

# Define function to compute accuracy and perform cross validation
def compute_accuracy(dataset, model, data_iterations, cv_iterations):

        #For each 'data_iteration', sample a new subset of data
        average_scores = []
```

```
        #Also keep track of all cross validation scores in order to compute confidence interval
        all_scores = []

        for i in range(0, data_iterations):

        #Split into labels (y) and features (X)
         X = data.drop("Normalized_Sel.", axis = 1)
          y = data["Normalized_Sel."]

        #Do N fold cross validation on selected training set
         Cv_scores = cross_val_score(model, X, y, cv = cv_iterations, scoring =
         'neg_mean_squared_error')
        accuracies = []
        for i in range(len(cv_scores)):
         cv_scores[i] = np.abs(cv_scores[i])
         accuracies.append(np.sqrt(cv_scores[i]))

        #Average the cross validation scores and append to accuracy dataframe
        avg_score = np.mean(accuracies)
        average_scores.append(avg_score)

        #Add each cross validation score to 'all_scores'
        for score in average_scores:
         all_scores.append(score)

        #Compute the average score over all data iterations
         overall_average_score = np.mean(average_scores)
         print("RMSE: ", overall_average_score)

          #Compute confidence interval of the accuracies
          mean1, CI_lower1, CI_upper1 = mean_confidence_interval(all_scores)
          print("RMSE Upper Bound: " + str(CI_upper1) + '\n' + "RMSE Lower Bound: " + str(CI_lower1))

        #Return overall average accuracy
        return overall_average_score

# Random Forest Model
        #Create Regressor
        model = RandomForestRegressor(n_estimators=120)

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
        accuracy_df = accuracy_df.append({'Model': 'RF', 'RMSE': accuracy}, ignore_index=True)

# LASSO
```

```
        #Create Regressor
        model = Lasso()

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
        accuracy_df = accuracy_df.append({'Model': 'LASSO', 'RMSE': accuracy}, ignore_index=True)

# Elastic-Net
        #Create Regressor
        model = linear_model.ElasticNet()

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
        accuracy_df = accuracy_df.append({'Model': 'Elastic-Net', 'RMSE': accuracy}, ignore_index=True)

# Gaussian Process Regression
        #Create Regressor
        kernel = 1.0 * RBF(1.0)
        model = GaussianProcessRegressor(kernel=kernel)

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
        accuracy_df = accuracy_df.append({'Model': 'GPR', 'RMSE': accuracy}, ignore_index=True)

# Support Vector Regression, kernel = linear
        #Create Regressor
        model = SVR(kernel='linear')

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
        accuracy_df = accuracy_df.append({'Model': 'SVR-linear', 'RMSE': accuracy}, ignore_index=True)

# Support Vector Regression, kernel = radial basis function
        #Create Regressor
        model = SVR(kernel='rbf')

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
```

```
        accuracy_df = accuracy_df.append({'Model': 'SVR-rbf', 'RMSE': accuracy}, ignore_index=True)

# Logistic Regression (Ridge Regression)
        #Create Classifier
        model = Ridge()

        #Call compute accuracy function
        accuracy = compute_accuracy(data, model, data_iterations=10, cv_iterations=20)

        #Track accuracy of each model in a dataframe
        accuracy_df = accuracy_df.append({'Model': 'Ridge', 'RMSE': accuracy}, ignore_index=True)
```

Hyperparameter Optimization

```
# Import Required Packages
        import numpy as np
        import pandas as pd
        from sklearn.model_selection import train_test_split
        from sklearn.ensemble import RandomForestRegressor
        from sklearn.model_selection import GridSearchCV
        from sklearn.model_selection import cross_val_score
        import scipy.stats

#Read in data and remove non-essential columns
        data = pd.read_csv("dataset.csv")
        data = data.drop("Catalyst", axis = 1)

#Hyperparameter Grid Search
        #Prevent warnings
        from warnings import filterwarnings
        filterwarnings('ignore')

        #Make Parameter Grid
        parameters = {
                'n_estimators':(20, 30, 50, 70, 100, 120, 150, 180, 210),
                 'criterion':('mse', 'mae'),
                'max_depth':(5, 10, 20, 30, 40, 50, 75, 100, 125),
                  'max_features':(3, 5, 7, 9, 10, 12, 14)
                }

        #Create training/test labels and features
                X = data.drop("Normalized Sel.", axis = 1)
                y = data["Normalized Sel."]
                X_train, X_test, y_train, y_test = train_test_split(X, y)

        #Create the classifier
                rf = RandomForestRegressor()
```

```
        #Call the GridSearch Cross Validation method on the model, with the given parameter grid
                clf = GridSearchCV(rf, parameters, cv=5)
                clf.fit(X_train, y_train)

        #Predict on the test set
                predictions = clf.predict(X_test)

                test_set = clf.predict(X_test)
                y_values = pd.Series(y_test).values
                sumall = 0
                for i in range(len(y_test)):
                  sum = test_set[i] - y_values[i]
                  sumall = sumall + sum**2
                rmse = np.sqrt(sumall/len(y_test))
                print(rmse)

        # List Optimal Parameters
                print(clf.best_params_)
                best_rf = clf.best_estimator_

# Cross Validate optimized model

        def compute_accuracy(dataset, model, data_iterations, cv_iterations):

        #For each 'data_iteration', sample a new subset of data
                average_scores = []

         #Also keep track of all cv scores in order to compute confidence interval
                all_scores = []

         for i in range(0, data_iterations):

         #Split into labels (y) and features (X)
                X = data.drop("Normalized Sel.", axis = 1)
                y = data["Normalized Sel."]

         #Do N fold cross validation on selected training set
                 cv_scores = cross_val_score(model, X, y, cv = cv_iterations, scoring =
                 'neg_mean_squared_error')
                 accuracies = []
                for i in range(len(cv_scores)):
                cv_scores[i] = np.abs(cv_scores[i])
                accuracies.append(np.sqrt(cv_scores[i]))

        #Average the cross validation scores, record it
                avg_score = np.mean(accuracies)
                average_scores.append(avg_score)
```

```
        #Add each cv score to 'all_scores'
                for score in average_scores:
                all_scores.append(score)

        #Compute the average score over all data iterations
                 overall_average_score = np.mean(average_scores)
                 print("RMSE: ", overall_average_score)

         #Compute confidence interval of the accuracies
                mean1, CI_lower1, CI_upper1 = mean_confidence_interval(all_scores)
                print("RMSE Upper Bound: " + str(CI_upper1) + '\n' + "RMSE Lower Bound: " +
                str(CI_lower1))

         #Return overall average accuracy
                 return overall_average_score
```

Catalyst Selectivity Predictions

```
# Import Required Packages

        import numpy as np
        import pandas as pd
        from sklearn.model_selection import train_test_split
        from sklearn.ensemble import RandomForestRegressor
        import sklearn.model_selection
        import scipy.stats

# Define mean confidence interval
        def mean_confidence_interval(data, confidence=0.95):
            a = 1.0 * np.array(data)
            n = len(a)
            m, se = np.mean(a), scipy.stats.sem(a)
            h = se * scipy.stats.t.ppf((1 + confidence) / 2., n-1)
            return m, m-h, m+h

# Read in data and remove non-essential columns
        #Read in data from csv
        data = pd.read_csv("dataset_maley.csv")


        #Remove non-essential column
        rows = data["Catalyst"]
        data = data.drop("Catalyst", axis = 1)

        # Predict Selectivity

        data_iterations = 10
        cv_iterations = 20
```

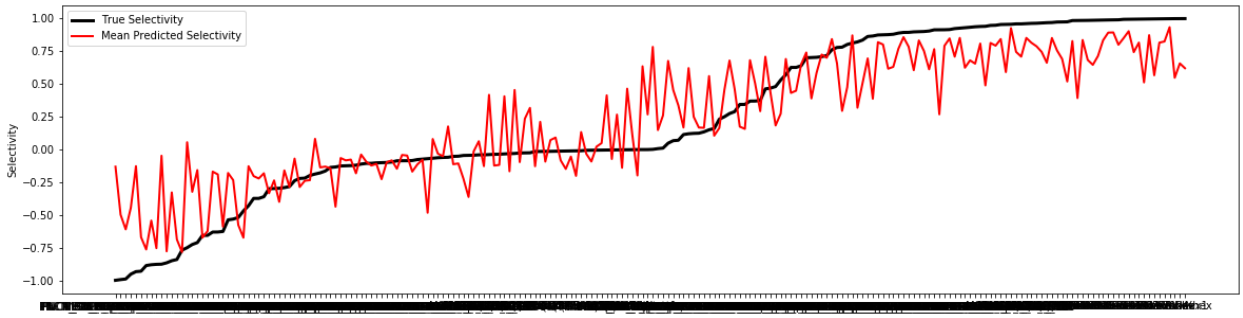
```
#Create training/test labels and features, remove unnecessary column
X = data.drop("Normalized Sel.", axis = 1)
y = data["Normalized Sel."]

#Create the Regressor
rf = RandomForestRegressor(criterion='mse',n_estimators=30,max_depth=40, max_features=3)

predictions_all = []
rmse_all = []
for i in range(0, data_iterations):
    for i in range(0, cv_iterations):
        X_train, X_test, y_train, y_test = train_test_split(X, y)

        rf.fit(X_train, y_train)
        predictions = rf.predict(X_test)

        y_values = pd.Series(y_test).values
        for i in range(len(y_values)):
            predictions_all.append([y_values[i],predictions[i]])

        sumall = 0
        for i in range(len(y_values)):
            sum = predictions[i] - y_values[i]
            sumall = sumall + sum**2
        rmse_all.append(np.sqrt(sumall/len(y_values)))

# Combine predictions by observation #
predictions_all.sort(key=lambda x: x[0])
key = 0
address = 0
for i in range(len(predictions_all)):
    if predictions_all[i][0] != key:
        key = predictions_all[i][0]
        address = i
        continue
    else:
        predictions_all[address].append(predictions_all[i][1])
        predictions_all[i].pop(1)
        predictions_all[i].pop(0)
        continue
predictions_all = [x for x in predictions_all if x != []]
true_y = []
pred_y = []
for i in range(len(predictions_all)):
    true_y.append(predictions_all[i][0])
    pred_y.append(predictions_all[i][1:])
```

```
pred_mean = []
pred_upper = []
pred_lower = []
for i in pred_y:
   mean, CI_lower, CI_upper = mean_confidence_interval(i)
   pred_mean.append(mean)
   pred_upper.append(CI_upper)
   pred_lower.append(CI_lower)

# output
mean1, CI_lower1, CI_upper1 = mean_confidence_interval(rmse_all)
print("RMSE Upper Bound: " + str(CI_upper1) + '\n' + "RMSE Mean: " + str(mean1) + '\n' +
"RMSE Lower Bound: " + str(CI_lower1))
```

Feature Importance From Optimized Random Forest Model

```
# Import Required Packages
import numpy as np
import pandas as pd
import seaborn as sns
from sklearn.ensemble import RandomForestRegressor

# Define Mean Confidence Interval
def mean_confidence_interval(data, confidence=0.95):
   a = 1.0 * np.array(data)
   n = len(a)
   m, se = np.mean(a), scipy.stats.sem(a)
   h = se * scipy.stats.t.ppf((1 + confidence) / 2., n-1)
   return m, m-h, m+h

# Read in data and remove non-essential columns
data = pd.read_csv('dataset.csv')
dataset = data.drop('Catalyst', axis = 1)

features_130 = dataset.drop("Normalized Selectivity", axis = 1)
labels_130 = dataset['Normalized Selectivity']

# Define Method to Compute Feature Importance
def calc_feature_importances(data, model, data_iterations, cv_iterations):

#Track overall average feature importances
      overall_average_importances = []
      for i in range(0, len(data.columns)-1):
         overall_average_importances.append([])

 #Iterate through data selection iterations
      importances_all = []
     for i in range(0, data_iterations):
```

```
            #Split into labels (y) and features (X)
                X = data.drop("Normalized Selectivity", axis = 1)
                y = data["Normalized Selectivity"]

            #Track importances at each iteration
                cv_importances = []
                for i in range(0, len(X.columns)):
                    cv_importances.append([])

            #Do N fold training on selected subset, record feature importances
                for i in range(0, cv_iterations):
                        model.fit(X, y)
                        importances = list(model.feature_importances_)
                        importances_all.append(model.feature_importances_)
                        for j in range(0, len(importances)):
                                cv_importances[j].append(importances[j])

            #Average importances
                avg_importances = []
                for list_of_importances in cv_importances:
                    avg_importances.append(np.mean(list_of_importances))

            #Record Averages
            for avg_imp in range(0, len(avg_importances)):
                overall_average_importances[avg_imp].append(avg_importances[avg_imp])


        #Compute the average score over all data iterations (samplings of 'other' trajectories for the
        training set)
        final_average_importances = []
        for q in overall_average_importances:
            final_average_importances.append(np.mean(q))

    #Return overall average feature importances
    return final_average_importances, importances_all

#Use Random Forest model to determine feature importances
    RF = RandomForestRegressor(criterion='mse',n_estimators=30,max_depth=40, max_features=3)

    #Call calc_feature_importances method to iteratively determine feature importances
        results, importances = calc_feature_importances(dataset, RF, 10, 20)

    #Display Results
        results
```



SI-Figure 1: Machine learning mean predicted selectivities (red) compared to DFT computed selectivities (black)

XYZ Coordinates and Thermochemistry

All optimized structures are cationic with a quartet spin state. All values reported computed at M06-L/6-31G** [LANL2DZ] level of theory. All energy values in Hartrees.

Ligands Used In Machine Learning Dataset

L1 – Hexene TS

Electronic Energy: -1620.69017557
Enthalpy: -1620.366800
Free Energy: -1620.444962

Cr	-1.470072	-0.539178	-0.419897
P	-0.135469	1.351095	0.241754
N	1.465026	0.776232	0.182370
C	1.579906	-0.518966	-0.259647
N	0.514174	-1.240899	-0.530235
H	2.291205	1.339492	0.345160
C	-0.234642	2.139839	1.943719
C	-0.005874	2.896354	-0.822221
C	1.013075	-2.578892	-0.901210
C	2.519610	-2.395684	-1.129312
H	3.119942	-3.204727	-0.710468
H	2.770115	-2.285072	-2.190915
H	0.496343	-2.953112	-1.787392
H	-2.765897	-1.468356	-0.784647
H	-2.566667	1.401024	-1.887768
H	-3.127817	1.629896	-0.165159
C	-3.565142	-0.329304	-1.002630
C	-2.856086	0.922932	-0.951038
C	-4.577654	-0.652584	0.088200
H	-4.331971	-0.055048	0.978279
H	-5.566358	-0.313422	-0.242029
C	-4.617220	-2.127272	0.477342
H	-4.894841	-2.735539	-0.395172
H	-5.404550	-2.283914	1.220611
C	-3.278835	-2.608675	1.031846
H	-3.008564	-1.978070	1.893999
H	-3.379914	-3.624700	1.434471
C	-2.147739	-2.577370	0.009530
H	-1.186980	-2.810198	0.479799
H	-2.302542	-3.308552	-0.793275
H	-3.849767	-0.673552	-2.002082
H	0.818240	-3.281816	-0.082200
F	-0.200153	1.172354	2.869065
F	-1.386545	2.809719	2.059478
F	0.781105	2.980206	2.176484
F	0.039142	2.524634	-2.110900
F	1.107004	3.595740	-0.555687
F	-1.067342	3.684316	-0.635890
N	2.760531	-1.139132	-0.417878
H	3.630702	-0.635586	-0.503979

L1 – Octene TS
Electronic Energy: -1699.29777526
Enthalpy: -1698.913076
Free Energy: -1698.996357

24	-1.342699	-0.572720	0.435854
15	0.050669	1.384903	0.140192
7	1.558630	0.766920	-0.332933
6	1.653260	-0.605248	-0.390630
7	0.612559	-1.369906	-0.174004

1	2.366935	1.342674	-0.537778
6	0.527647	2.570878	1.514946
6	-0.320727	2.605357	-1.238540
6	1.112024	-2.753411	-0.216930
6	2.520520	-2.659251	-0.825010
1	3.251851	-3.290881	-0.318088
1	2.528430	-2.903665	-1.893987
1	0.450559	-3.391475	-0.809231
6	-2.288343	-2.505966	0.333121
6	-2.506760	-1.952601	-1.086429
6	-3.963333	-1.734473	-1.469028
6	-4.717555	-0.756128	-0.579351
6	-3.002615	0.678359	0.655188
6	-4.053549	0.613454	-0.443199
1	-3.214807	-2.964310	0.673052
1	-1.956282	-1.005664	-1.349690
1	-4.466333	-2.708490	-1.463234
1	-5.728918	-0.646653	-0.983854
1	-2.680094	1.718972	0.800992
1	-1.494982	-3.254629	0.341146
1	-2.015185	-2.646106	-1.778009
1	-4.846407	-1.188510	0.424544
1	-3.455098	0.380025	1.612792
1	-3.630877	0.917327	-1.414617
1	-4.831859	1.360053	-0.231542
6	-1.109119	-0.769638	2.458379
1	-1.489880	0.143876	2.912777
1	-0.086274	-1.036478	2.721901
6	-2.037003	-1.830337	2.219270
1	-3.082959	-1.630979	2.437735
1	-1.728253	-2.841034	2.471201
1	1.139260	-3.161043	0.802856
9	-0.536284	3.266909	1.921377
9	1.482296	3.427089	1.118863
9	-1.236660	3.492971	-0.844236
9	-0.805554	1.917385	-2.285601
9	0.775101	3.260366	-1.645560
9	1.003138	1.858864	2.544215
1	-3.995050	-1.379715	-2.506395
7	2.819013	-1.240943	-0.621372
1	3.598954	-0.792116	-1.078069

L2 – Hexene TS

Electronic Energy: -1659.99545673
Enthalpy: -1659.642404
Free Energy: -1659.723445

Cr	-1.451731	-0.554823	-0.420775
P	-0.122585	1.302666	0.287143
N	1.472674	0.711366	0.308977
C	1.592890	-0.576432	-0.156987
N	0.524891	-1.261999	-0.519292
H	2.294514	1.286501	0.450233
C	-0.309203	2.080180	1.985757
C	0.081436	2.854751	-0.753082
C	1.012387	-2.600149	-0.900571
C	2.530029	-2.445081	-1.027107
H	3.093659	-3.274142	-0.593123
H	2.857545	-2.309891	-2.066886
H	0.542679	-2.931161	-1.829080
H	-2.758624	-1.467482	-0.786488
H	-2.520036	1.407264	-1.878368
H	-3.084808	1.633712	-0.156800
C	-3.542004	-0.316735	-1.007874
C	-2.818947	0.927514	-0.945379
C	-4.565319	-0.634696	0.074500

H	-4.317719	-0.046639	0.970400
H	-5.547674	-0.280937	-0.259296
C	-4.625138	-2.111683	0.452232
H	-4.899275	-2.710271	-0.428095
H	-5.422514	-2.265659	1.185316
C	-3.298250	-2.611091	1.018435
H	-3.032231	-1.989327	1.888137
H	-3.414732	-3.628917	1.412294
C	-2.153449	-2.583396	0.010870
H	-1.200485	-2.816880	0.496771
H	-2.297111	-3.316097	-0.792646
H	-3.824951	-0.651214	-2.011073
H	0.751645	-3.326156	-0.120664
F	-0.279297	1.108940	2.907800
F	-1.486592	2.711624	2.060662
F	0.668639	2.951840	2.262399
F	0.166506	2.495982	-2.042974
F	1.200066	3.526044	-0.438719
F	-0.968390	3.664471	-0.595580
N	2.769619	-1.211204	-0.273227
C	4.084921	-0.618514	-0.189665
H	4.370041	-0.109468	-1.118813
H	4.140776	0.086609	0.642689
H	4.811672	-1.406739	0.010114

L2 – Octene TS

Electronic Energy: -1738.60250020
Enthalpy: -1738.188634
Free Energy: -1738.274523

Cr	-1.343442	-0.565534	0.430795
P	0.075669	1.370602	0.218068
N	1.588474	0.754492	-0.241189
C	1.677492	-0.619156	-0.295684
N	0.619021	-1.373693	-0.105817
H	2.370189	1.330990	-0.528203
C	0.487869	2.468302	1.687766
C	-0.194291	2.693093	-1.088694
C	1.108720	-2.760777	-0.117420
C	2.527280	-2.679428	-0.691034
H	3.251075	-3.306884	-0.165670
H	2.566338	-2.928884	-1.760518
H	0.458423	-3.400806	-0.719406
C	-2.272259	-2.501981	0.350084
C	-2.462704	-1.990768	-1.087678
C	-3.914518	-1.794113	-1.498030
C	-4.680300	-0.789416	-0.648363
C	-2.997135	0.711738	0.559482
C	-4.023041	0.588013	-0.558229
H	-3.199767	-2.963454	0.682667
H	-1.915313	-1.045342	-1.365898
H	-4.413225	-2.769874	-1.465170
H	-5.689536	-0.699803	-1.062844
H	-2.678017	1.759550	0.652011
H	-1.467190	-3.235986	0.405488
H	-1.952014	-2.698999	-1.750260
H	-4.814125	-1.186546	0.369440
H	-3.471088	0.468579	1.522202
H	-3.575639	0.847079	-1.531582
H	-4.808071	1.341285	-0.401714
C	-1.171226	-0.699120	2.472808
H	-1.561619	0.231870	2.880647
H	-0.158175	-0.960426	2.776002
C	-2.094088	-1.760765	2.236013
H	-3.147746	-1.553759	2.405574
H	-1.798147	-2.765931	2.522693

H	1.109335	-3.157546	0.907373
F	-0.627387	3.025947	2.167836
F	1.355008	3.440371	1.368342
F	-1.003679	3.650416	-0.629042
F	-0.756683	2.126770	-2.167024
F	0.964311	3.253792	-1.470129
F	1.040113	1.710130	2.644278
H	-3.936008	-1.473595	-2.546661
N	2.842649	-1.262022	-0.499248
C	4.075255	-0.684622	-0.981626
H	4.056038	-0.498987	-2.063161
H	4.301101	0.247323	-0.457484
H	4.891825	-1.374923	-0.765580

L3 – Hexene TS
Electronic Energy: -1213.40828028
Enthalpy: -1212.969178
Free Energy: -1213.046795

Cr	-1.451731	-0.554823	-0.420775
P	-0.122585	1.302666	0.287143
N	1.472674	0.711366	0.308977
C	1.592890	-0.576432	-0.156987
N	0.524891	-1.261999	-0.519292
H	2.294514	1.286501	0.450233
C	-0.309203	2.080180	1.985757
C	0.081436	2.854751	-0.753082
C	1.012387	-2.600149	-0.900571
C	2.530029	-2.445081	-1.027107
H	3.093659	-3.274142	-0.593123
H	2.857545	-2.309891	-2.066886
H	0.542679	-2.931161	-1.829080
H	-2.758624	-1.467482	-0.786488
H	-2.520036	1.407264	-1.878368
H	-3.084808	1.633712	-0.156800
C	-3.542004	-0.316735	-1.007874
C	-2.818947	0.927514	-0.945379
C	-4.565319	-0.634696	0.074500
H	-4.317719	-0.046639	0.970400
H	-5.547674	-0.280937	-0.259296
C	-4.625138	-2.111683	0.452232
H	-4.899275	-2.710271	-0.428095
H	-5.422514	-2.265659	1.185316
C	-3.298250	-2.611091	1.018435
H	-3.032231	-1.989327	1.888137
H	-3.414732	-3.628917	1.412294
C	-2.153449	-2.583396	0.010870
H	-1.200485	-2.816880	0.496771
H	-2.297111	-3.316097	-0.792646
H	-3.824951	-0.651214	-2.011073
H	0.751645	-3.326156	-0.120664
F	-0.279297	1.108940	2.907800
F	-1.486592	2.711624	2.060662
F	0.668639	2.951840	2.262399
F	0.166506	2.495982	-2.042974
F	1.200066	3.526044	-0.438719
F	-0.968390	3.664471	-0.595580
N	2.769619	-1.211204	-0.273227
C	4.084921	-0.618514	-0.189665
H	4.370041	-0.109468	-1.118813
H	4.140776	0.086609	0.642689
H	4.811672	-1.406739	0.010114

L3 – Octene TS
Electronic Energy: -1292.01714086
Enthalpy: -1291.516884

Free Energy: -1291.598222

Cr	-1.343442	-0.565534	0.430795
P	0.075669	1.370602	0.218068
N	1.588474	0.754492	-0.241189
C	1.677492	-0.619156	-0.295684
N	0.619021	-1.373693	-0.105817
H	2.370189	1.330990	-0.528203
C	0.487869	2.468302	1.687766
C	-0.194291	2.693093	-1.088694
C	1.108720	-2.760777	-0.117420
C	2.527280	-2.679428	-0.691034
H	3.251075	-3.306884	-0.165670
H	2.566338	-2.928884	-1.760518
H	0.458423	-3.400806	-0.719406
C	-2.272259	-2.501981	0.350084
C	-2.462704	-1.990768	-1.087678
C	-3.914518	-1.794113	-1.498030
C	-4.680300	-0.789416	-0.648363
C	-2.997135	0.711738	0.559482
C	-4.023041	0.588013	-0.558229
H	-3.199767	-2.963454	0.682667
H	-1.915313	-1.045342	-1.365898
H	-4.413225	-2.769874	-1.465170
H	-5.689536	-0.699803	-1.062844
H	-2.678017	1.759550	0.652011
H	-1.467190	-3.235986	0.405488
H	-1.952014	-2.698999	-1.750260
H	-4.814125	-1.186546	0.369440
H	-3.471088	0.468579	1.522202
H	-3.575639	0.847079	-1.531582
H	-4.808071	1.341285	-0.401714
C	-1.171226	-0.699120	2.472808
H	-1.561619	0.231870	2.880647
H	-0.158175	-0.960426	2.776002
C	-2.094088	-1.760765	2.236013
H	-3.147746	-1.553759	2.405574
H	-1.798147	-2.765931	2.522693
H	1.109335	-3.157546	0.907373
F	-0.627387	3.025947	2.167836
F	1.355008	3.440371	1.368342
F	-1.003679	3.650416	-0.629042
F	-0.756683	2.126770	-2.167024
F	0.964311	3.253792	-1.470129
F	1.040113	1.710130	2.644278
H	-3.936008	-1.473595	-2.546661
N	2.842649	-1.262022	-0.499248
C	4.075255	-0.684622	-0.981626
H	4.056038	-0.498987	-2.063161
H	4.301101	0.247323	-0.457484
H	4.891825	-1.374923	-0.765580

L4 – Hexene TS
Electronic Energy: -1252.76803048
Enthalpy: -1252.299272
Free Energy: -1252.376684

Cr	-1.373440	-0.537353	-0.573599
P	-0.109721	1.403841	0.102646
N	1.527607	0.769066	-0.035977
C	1.626872	-0.554870	-0.325223
N	0.555405	-1.295945	-0.538542
H	2.365032	1.327328	0.062428
C	1.032473	-2.677317	-0.713651
C	2.537218	-2.542121	-0.973037
H	3.131082	-3.317745	-0.486516

H	2.772514	-2.541324	-2.044848
H	0.506648	-3.172703	-1.532904
H	-2.679191	-1.494059	-0.808249
H	-2.343039	1.152585	-2.391968
H	-2.954627	1.676642	-0.752756
C	-3.427675	-0.380714	-1.278299
C	-2.677676	0.843681	-1.401284
C	-4.504236	-0.486281	-0.204672
H	-4.282182	0.252264	0.580218
H	-5.464797	-0.186973	-0.639766
C	-4.609542	-1.868286	0.434323
H	-4.852657	-2.617115	-0.332826
H	-5.443966	-1.878581	1.141639
C	-3.319702	-2.266582	1.148577
H	-3.081001	-1.490121	1.893200
H	-3.474843	-3.186961	1.725399
C	-2.134002	-2.445748	0.202908
H	-1.202418	-2.597295	0.759722
H	-2.265281	-3.318872	-0.447734
H	-3.678462	-0.882896	-2.218132
H	0.838180	-3.255553	0.199469
C	-0.302230	3.974348	0.522659
C	-0.038959	3.321997	1.864142
H	0.281538	4.890170	0.382998
H	-1.368371	4.228923	0.411949
H	1.024825	3.394988	2.145709
H	-0.632191	3.768477	2.667467
N	-0.446187	1.930709	1.662030
N	0.106749	2.976797	-0.468903
C	-0.363179	1.017947	2.786579
H	-0.723379	0.027884	2.485257
H	0.662316	0.906989	3.167254
H	-0.999293	1.373026	3.601612
C	-0.119629	3.310490	-1.865142
H	-1.173913	3.533487	-2.080067
H	0.478043	4.186330	-2.133056
H	0.197841	2.483668	-2.505313
N	2.801079	-1.227700	-0.383609
H	3.674847	-0.751571	-0.544624

L4 – Octene TS

Electronic Energy: -1331.32155051
Enthalpy: -1330.792159
Free Energy: -1330.877318

Cr	-1.267225	-0.542762	0.472604
P	0.060096	1.452670	0.046570
N	1.612947	0.718369	-0.313758
C	1.668827	-0.642926	-0.382230
N	0.600937	-1.396422	-0.255461
H	2.475593	1.245735	-0.343684
C	1.072633	-2.786566	-0.287505
C	2.513280	-2.715532	-0.812723
H	3.195397	-3.391669	-0.293979
H	2.569243	-2.923428	-1.888767
H	0.434442	-3.406308	-0.924812
C	-2.289440	-2.453134	0.261269
C	-2.539677	-1.779591	-1.098248
C	-4.000840	-1.489770	-1.411456
C	-4.689454	-0.558183	-0.422922
C	-2.886694	0.707153	0.867644
C	-3.967135	0.771880	-0.202763
H	-3.222439	-2.894084	0.607353
H	-1.978084	-0.821082	-1.294924
H	-4.536533	-2.444698	-1.464595
H	-5.708261	-0.382700	-0.782615

H	-2.507506	1.718344	1.077886
H	-1.535545	-3.235126	0.169742
H	-2.085644	-2.418316	-1.864626
H	-4.055524	-1.054182	-2.417078
H	-4.804918	-1.063121	0.548127
H	-3.331123	0.354942	1.811263
H	-3.547739	1.127067	-1.159253
H	-4.711133	1.531444	0.075011
C	-0.944197	-0.924022	2.455596
H	-1.286969	-0.056145	3.015200
H	0.085621	-1.230279	2.637780
C	-1.907770	-1.945212	2.177145
H	-2.933688	-1.742284	2.472889
H	-1.614554	-2.980127	2.330213
H	1.036211	-3.211777	0.726170
C	0.066652	4.012140	0.567526
C	0.107807	3.862027	-0.939092
H	0.748066	4.790171	0.927263
H	-0.950001	4.261403	0.909535
H	1.133927	3.979179	-1.327007
H	-0.530015	4.591349	-1.447022
N	-0.404080	2.510921	-1.171914
N	0.493756	2.709954	1.085863
C	-0.542699	2.058582	-2.541392
H	0.414947	2.038198	-3.081891
H	-0.963229	1.047503	-2.556538
H	-1.231405	2.714420	-3.080981
C	0.454940	2.528636	2.527740
H	1.104580	3.268192	3.003589
H	-0.557210	2.639428	2.942806
H	0.832916	1.537136	2.789175
N	2.841244	-1.316459	-0.534473
H	3.630703	-0.881316	-0.986665

L5 – Hexene TS

Electronic Energy: -1102.77268624
Enthalpy: -1102.369226
Free Energy: -1102.438961

Cr	-1.285562	-0.595232	-0.538822
P	0.033388	1.317324	0.140395
N	1.654212	0.661425	-0.024261
C	1.732465	-0.633888	-0.427360
N	0.642805	-1.342244	-0.678928
H	2.503861	1.171565	0.181719
C	1.096176	-2.697601	-1.026782
C	2.597972	-2.555312	-1.280135
H	3.193001	-3.373295	-0.866835
H	2.837201	-2.461187	-2.349403
H	0.557872	-3.077236	-1.898528
H	-2.619202	-1.520176	-0.752783
H	-2.412129	1.311744	-2.023399
H	-2.894092	1.591752	-0.289840
C	-3.397808	-0.385092	-1.055981
C	-2.666732	0.857631	-1.065362
C	-4.410468	-0.654957	0.050499
H	-4.148997	-0.033225	0.919934
H	-5.397464	-0.311628	-0.281924
C	-4.470055	-2.116805	0.487431
H	-4.742726	-2.748073	-0.370670
H	-5.269583	-2.243981	1.224160
C	-3.144169	-2.596588	1.075409
H	-2.887798	-1.943753	1.924664
H	-3.264927	-3.600633	1.502568
C	-1.991340	-2.594190	0.072761
H	-1.038201	-2.780325	0.579805

H	-2.113700	-3.378717	-0.684653
H	-3.698429	-0.769044	-2.036273
H	0.897417	-3.385418	-0.194250
C	0.436464	3.851321	0.495695
C	-0.224548	3.354376	1.763613
N	-0.073488	1.899314	1.721146
N	0.059242	2.865229	-0.521108
C	-0.783262	1.128837	2.725324
H	-0.593420	0.060181	2.578524
H	-0.421245	1.392072	3.723624
H	-1.871332	1.298013	2.698828
C	0.566464	3.076140	-1.862828
H	0.201109	4.032040	-2.247480
H	1.666820	3.084849	-1.903910
H	0.206645	2.285667	-2.527486
N	2.897382	-1.299910	-0.590488
C	4.207721	-0.700025	-0.664167
H	4.386121	-0.192449	-1.621786
H	4.355630	0.010197	0.153158
H	4.958140	-1.483328	-0.545842
H	1.532659	3.911450	0.612091
H	0.076166	4.840941	0.199702
H	0.251897	3.755799	2.664389
H	-1.289987	3.633559	1.784332

L5 – Octene TS

Electronic Energy: -1181.32497248
Enthalpy: -1180.860549
Free Energy: -1180.936007

Cr	-1.259838	-0.543571	0.491901
P	0.075948	1.449423	0.109275
N	1.640495	0.717120	-0.188587
C	1.695956	-0.642750	-0.284836
N	0.613161	-1.389031	-0.213403
H	2.494006	1.252981	-0.273047
C	1.076497	-2.781622	-0.247638
C	2.526265	-2.707248	-0.731565
H	3.198555	-3.398897	-0.217778
H	2.615965	-2.881171	-1.814332
H	0.452446	-3.388980	-0.910029
C	-2.281042	-2.451879	0.255838
C	-2.510754	-1.772654	-1.104329
C	-3.966934	-1.480370	-1.437645
C	-4.667994	-0.549412	-0.457256
C	-2.884133	0.709277	0.865253
C	-3.945884	0.778531	-0.223566
H	-3.219267	-2.893480	0.586700
H	-1.945646	-0.813984	-1.288267
H	-4.503289	-2.434392	-1.500157
H	-5.681125	-0.371042	-0.831348
H	-2.508534	1.719836	1.085025
H	-1.526480	-3.234194	0.172491
H	-2.046173	-2.408465	-1.866834
H	-4.006793	-1.042765	-2.443090
H	-4.798491	-1.056207	0.510930
H	-3.345215	0.355011	1.800163
H	-3.508070	1.132841	-1.172231
H	-4.692567	1.540148	0.041221
C	-0.968136	-0.932843	2.478835
H	-1.319049	-0.066566	3.035848
H	0.058528	-1.240557	2.675939
C	-1.928165	-1.951596	2.180876
H	-2.958522	-1.748671	2.460817
H	-1.638763	-2.987650	2.333527
H	1.012359	-3.220427	0.759328

C	0.045432	4.013593	0.607312
C	0.138204	3.852468	-0.895941
H	0.707041	4.801069	0.983252
H	-0.984445	4.255895	0.913014
H	1.175540	3.977598	-1.250349
H	-0.489520	4.571548	-1.430470
N	-0.352309	2.494830	-1.134429
N	0.467559	2.719898	1.149489
C	-0.445046	2.029918	-2.503236
H	0.528977	2.011568	-3.014062
H	-0.857652	1.015625	-2.522394
H	-1.120966	2.676098	-3.070072
C	0.385891	2.549740	2.590771
H	1.010278	3.302012	3.080373
H	-0.640146	2.649644	2.973402
H	0.769164	1.565729	2.872060
N	2.867066	-1.319769	-0.415268
C	4.111850	-0.743806	-0.866821
H	4.121385	-0.546757	-1.947586
H	4.323296	0.184247	-0.330353
H	4.925489	-1.433078	-0.635999

L6 – Hexene
Electronic Energy: -1142.07605832
Enthalpy: -1141.643339
Free Energy: -1141.717769

Cr	-1.433900	-0.522463	-0.445308
P	-0.092622	1.397053	0.223874
N	1.506013	0.719603	0.194811
C	1.589178	-0.590344	-0.157405
N	0.518199	-1.297836	-0.458447
H	2.356217	1.236500	0.375989
C	0.985664	-2.671797	-0.703969
C	2.505208	-2.551204	-0.865410
H	3.055197	-3.362565	-0.385170
H	2.806548	-2.501271	-1.919309
H	0.500926	-3.097071	-1.585870
H	-2.732747	-1.445788	-0.813097
H	-2.463160	1.451413	-1.914494
H	-3.110381	1.629589	-0.218267
C	-3.493424	-0.307800	-1.134762
C	-2.788719	0.944366	-1.005602
C	-4.611702	-0.639028	-0.154546
H	-4.454357	-0.050951	0.761587
H	-5.563335	-0.295650	-0.577098
C	-4.689569	-2.116926	0.217264
H	-4.863124	-2.719051	-0.686238
H	-5.555874	-2.283908	0.864949
C	-3.419136	-2.594641	0.916756
H	-3.255669	-1.964702	1.805095
H	-3.561055	-3.612884	1.301622
C	-2.176520	-2.546382	0.030869
H	-1.274772	-2.740604	0.621031
H	-2.214968	-3.303987	-0.761804
H	-3.690073	-0.636640	-2.160374
H	0.728874	-3.310619	0.151111
C	-0.210875	4.104472	0.340168
C	0.304340	3.619929	1.690731
H	0.241796	5.051254	0.034446
H	-1.292763	4.273945	0.401653
H	1.402577	3.601590	1.688170
H	-0.000442	4.274568	2.511531
N	2.756014	-1.275493	-0.195124
H	3.640709	-0.801701	-0.297478
C	0.080284	3.001170	-0.681151

C	-0.241300	2.204903	1.871707
H	1.109033	3.061481	-1.053110
H	-0.578280	3.031748	-1.551845
H	0.256555	1.608354	2.639939
H	-1.308288	2.232760	2.122806

L6 – Octene

Electronic Energy: -1220.68283488
Enthalpy: -1220.187399
Free Energy: -1220.264565

Cr	-1.328641	-0.561817	0.388854
P	0.004897	1.437766	0.015906
N	1.558259	0.746822	-0.334443
C	1.641632	-0.615402	-0.375871
N	0.591467	-1.387739	-0.233189
H	2.407215	1.285257	-0.437269
C	0.324557	2.694403	1.335191
C	-0.266511	2.701167	-1.293646
C	1.096862	-2.767048	-0.233766
C	2.530795	-2.673005	-0.772711
H	3.232294	-3.325803	-0.250118
H	2.581338	-2.895302	-1.846120
H	0.468813	-3.417744	-0.849406
C	-2.279864	-2.515397	0.302670
C	-2.548648	-1.952384	-1.103026
C	-4.019856	-1.738590	-1.430888
C	-4.739880	-0.762068	-0.510362
C	-2.988124	0.676924	0.664436
C	-4.071954	0.609534	-0.403578
H	-3.193707	-2.976876	0.672117
H	-2.016824	-0.994855	-1.370486
H	-4.520535	-2.713532	-1.409102
H	-5.767461	-0.656198	-0.871988
H	-2.659955	1.720170	0.797235
H	-1.488236	-3.264811	0.275801
H	-2.076627	-2.633282	-1.820710
H	-4.093585	-1.381979	-2.465590
H	-4.827353	-1.193459	0.498333
H	-3.419684	0.389030	1.635191
H	-3.671413	0.896215	-1.390602
H	-4.845123	1.359426	-0.185954
C	-1.028872	-0.782367	2.399677
H	-1.405777	0.116522	2.883568
H	0.005798	-1.041096	2.621400
C	-1.956812	-1.849894	2.185347
H	-2.994893	-1.657476	2.444068
H	-1.637047	-2.861252	2.420544
H	0.103383	2.352080	-2.260338
H	-0.281062	2.482778	2.219719
H	1.079219	-3.165332	0.791157
H	-1.351522	2.832515	-1.388500
H	1.372579	2.599981	1.638928
C	0.031830	4.064046	0.710830
C	0.385294	3.981096	-0.770730
H	0.580123	4.855981	1.226878
H	-1.034185	4.296409	0.817421
H	1.475110	3.926658	-0.896907
H	0.049018	4.859668	-1.327232
N	2.830112	-1.262662	-0.517333
H	3.608112	-0.819825	-0.981910

L7 – Hexene

Electronic Energy: -1025.35858719
Enthalpy: -1024.993785
Free Energy: -1025.061730

Cr	-1.438164	-0.583352	-0.443850
P	-0.121944	1.333776	0.263071
N	1.479014	0.660686	0.286818
C	1.581690	-0.626801	-0.140781
N	0.515642	-1.319024	-0.503643
H	2.322474	1.205240	0.409643
C	-0.331952	2.141994	1.904300
C	0.079414	2.939810	-0.635336
C	0.995855	-2.672615	-0.824052
C	2.509688	-2.522105	-0.973409
H	3.078450	-3.353764	-0.550452
H	2.817941	-2.389294	-2.020750
H	0.517792	-3.050899	-1.730313
H	-2.731661	-1.528138	-0.783216
H	-2.509924	1.343551	-1.937348
H	-3.129368	1.570563	-0.236891
C	-3.515494	-0.396284	-1.087066
C	-2.815352	0.863100	-1.007068
H	-1.406288	2.153498	2.123724
C	-4.592806	-0.714456	-0.057908
H	-4.403365	-0.108530	0.840513
H	-5.562754	-0.384227	-0.448253
C	-4.647870	-2.185596	0.344098
H	-4.857021	-2.804721	-0.540143
H	-5.485568	-2.343551	1.030486
C	-3.347296	-2.648033	0.997051
H	-3.145816	-2.001264	1.865770
H	-3.470287	-3.659128	1.406557
C	-2.145114	-2.613926	0.056612
H	-1.217663	-2.804310	0.606901
H	-2.219816	-3.379918	-0.725437
H	-3.747617	-0.747826	-2.097695
H	0.745951	-3.363008	-0.007554
H	0.150680	1.553421	2.688057
H	1.124919	3.010597	-0.955861
H	-0.532499	2.964912	-1.539607
C	-0.270460	4.039811	0.370278
C	0.199122	3.565038	1.741220
H	0.179562	4.992634	0.079474
H	-1.356242	4.193475	0.388507
H	1.296599	3.560215	1.780377
H	-0.145788	4.216530	2.548536
N	2.756377	-1.291216	-0.221714
C	4.067385	-0.690148	-0.174938
H	4.329325	-0.174572	-1.108924
H	4.139454	0.013638	0.658223
H	4.807182	-1.471670	0.004010

L7 – Octene

Electronic Energy: -1103.96568630
Enthalpy: -1103.539120
Free Energy: -1103.611433

Cr	-1.318855	-0.564517	0.477083
P	0.028409	1.439605	0.105290
N	1.562822	0.742989	-0.301732
C	1.661843	-0.617546	-0.282903
N	0.617130	-1.389650	-0.069562
H	2.386651	1.286514	-0.522425
C	0.394171	2.695213	1.411162
C	-0.269608	2.700316	-1.199088
C	1.129770	-2.764367	-0.016988
C	2.545827	-2.685324	-0.592834
H	3.275844	-3.295510	-0.055054
H	2.581811	-2.964099	-1.656442

H	0.493843	-3.445301	-0.589932
C	-2.274218	-2.504237	0.292937
C	-2.448658	-1.918431	-1.118332
C	-3.896332	-1.704679	-1.537654
C	-4.683679	-0.753899	-0.646084
C	-3.015853	0.647235	0.679175
C	-4.031817	0.615782	-0.454418
H	-3.216133	-2.953382	0.602895
H	-1.906287	-0.954354	-1.332639
H	-4.391212	-2.682759	-1.568136
H	-5.684202	-0.641210	-1.076923
H	-2.696907	1.684328	0.870731
H	-1.497126	-3.268895	0.300440
H	-1.928413	-2.585835	-1.814808
H	-3.904660	-1.325683	-2.567354
H	-4.838029	-1.211500	0.342966
H	-3.510715	0.325877	1.608948
H	-3.573937	0.934824	-1.405948
H	-4.823565	1.354310	-0.261711
C	-1.148262	-0.816191	2.501949
H	-1.560348	0.077186	2.967913
H	-0.126705	-1.068607	2.783428
C	-2.049682	-1.884834	2.208083
H	-3.103164	-1.710250	2.411185
H	-1.731824	-2.899514	2.432512
H	0.080198	2.344732	-2.171400
H	-0.180817	2.486994	2.317157
H	1.138115	-3.118358	1.023970
H	-1.354848	2.839049	-1.274535
H	1.452200	2.596594	1.676819
C	0.085556	4.063368	0.795263
C	0.398194	3.978685	-0.695071
H	0.649038	4.855576	1.295043
H	-0.977522	4.295750	0.929532
H	1.484094	3.920676	-0.849349
H	0.047283	4.857213	-1.243264
N	2.846395	-1.262433	-0.437766
C	4.036541	-0.692417	-1.020474
H	3.974788	-0.611359	-2.114425
H	4.238356	0.295899	-0.600232
H	4.891423	-1.323118	-0.770371

L8 – Hexene

Electronic Energy: -1064.66314677
Enthalpy: -1064.268790
Free Energy: -1064.340040

Cr	-1.446078	-0.505528	-0.427848
P	-0.113384	1.444480	0.210266
N	1.490932	0.823386	0.012272
C	1.586004	-0.490279	-0.321786
N	0.516268	-1.236834	-0.510310
H	2.337442	1.354295	0.168854
C	-0.154333	2.053816	1.921866
C	-0.080809	2.972840	-0.768241
C	1.007201	-2.598134	-0.783441
C	2.500481	-2.429114	-1.086292
H	3.119845	-3.214948	-0.650353
H	2.701036	-2.383542	-2.164093
H	0.457738	-3.054203	-1.609987
H	-2.734485	-1.464805	-0.750521
H	-2.564487	1.404017	-1.917077
H	-3.150743	1.624970	-0.203660
C	-3.537092	-0.344421	-1.038183
C	-2.847422	0.920923	-0.980959
H	0.727895	3.637755	-0.451471

H	-1.124749	2.520430	2.114540
C	-4.584187	-0.665402	0.020783
H	-4.372143	-0.057333	0.912811
H	-5.565763	-0.339056	-0.342956
C	-4.622644	-2.136069	0.425643
H	-4.853414	-2.756822	-0.451992
H	-5.440502	-2.296462	1.134979
C	-3.303193	-2.593225	1.043104
H	-3.082999	-1.949001	1.909233
H	-3.409975	-3.606554	1.451655
C	-2.125816	-2.549262	0.072330
H	-1.185232	-2.746717	0.596232
H	-2.221686	-3.307835	-0.714726
H	-3.789943	-0.706159	-2.040169
H	0.853951	-3.230406	0.100717
H	-0.031810	1.223495	2.620253
H	0.626573	2.796994	2.106805
H	0.042235	2.741632	-1.828327
H	-1.028527	3.503041	-0.642098
N	2.768110	-1.135133	-0.457342
H	3.615565	-0.627527	-0.663430

L8 – Octene

Electronic Energy: -1143.27001901
Enthalpy: -1142.814432
Free Energy: -1142.889461

Cr	-1.308992	-0.549949	0.440286
P	0.024573	1.457851	0.039430
N	1.514353	0.764096	-0.497923
C	1.615190	-0.596632	-0.493162
N	0.612560	-1.368580	-0.148431
H	2.318718	1.310346	-0.776397
C	0.493866	2.520804	1.433942
C	-0.417852	2.632761	-1.270453
C	1.089605	-2.751473	-0.275449
C	2.610427	-2.642883	-0.465915
H	3.157151	-2.831993	0.466284
H	2.996183	-3.315453	-1.234467
H	0.613176	-3.232905	-1.139966
C	-2.257289	-2.494275	0.241370
C	-2.490966	-1.870420	-1.144672
C	-3.953534	-1.660753	-1.509998
C	-4.715028	-0.734608	-0.571797
C	-3.006401	0.634467	0.735229
C	-4.058214	0.630629	-0.365877
H	-3.182115	-2.962511	0.573323
H	-1.971749	-0.891414	-1.349871
H	-4.442210	-2.641618	-1.545648
H	-5.728742	-0.613513	-0.967923
H	-2.688724	1.667409	0.946554
H	-1.471216	-3.248652	0.194311
H	-1.989081	-2.510863	-1.878429
H	-3.998780	-1.259504	-2.530253
H	-4.836269	-1.218203	0.409283
H	-3.467102	0.280600	1.670637
H	-3.629198	0.976122	-1.322063
H	-4.843665	1.362888	-0.129154
C	-1.060983	-0.849914	2.446796
H	-1.460124	0.027959	2.952601
H	-0.025749	-1.100417	2.675837
C	-1.963192	-1.921368	2.159800
H	-3.008870	-1.764226	2.411222
H	-1.626499	-2.937390	2.347904
H	-0.642026	2.097894	-2.196221
H	-0.398190	3.029489	1.811006

H	0.823848	-3.336029	0.611649
H	-1.315524	3.180133	-0.969100
H	0.904333	1.912009	2.242485
H	0.378362	3.358234	-1.459762
H	1.226254	3.279223	1.143440
N	2.747382	-1.243217	-0.870479
H	3.645676	-0.786376	-0.816433

L9 – Hexene
Electronic Energy: -1408.79922699
Enthalpy: -1408.320610
Free Energy: -1408.402406

Cr	-1.430152	-0.517594	-0.376850
P	-0.087731	1.396671	0.314538
N	1.508874	0.722673	0.268277
C	1.597223	-0.565929	-0.159639
N	0.517985	-1.259840	-0.476559
H	2.354828	1.267662	0.369839
C	-0.219909	2.098745	1.984719
C	0.052723	2.873609	-0.733630
C	0.985016	-2.616652	-0.803567
C	2.493733	-2.471339	-1.003629
H	3.074019	-3.299472	-0.589576
H	2.768452	-2.351510	-2.061734
H	0.477023	-2.999927	-1.691253
H	-2.715988	-1.465691	-0.731942
H	-2.496814	1.434313	-1.842432
H	-3.135552	1.615545	-0.143168
C	-3.500991	-0.332183	-1.037938
C	-2.809647	0.929534	-0.927390
H	0.860718	3.532434	-0.402469
H	-1.172546	2.628138	2.076680
C	-4.594936	-0.669111	-0.031957
H	-4.432069	-0.063324	0.871454
H	-5.560875	-0.350292	-0.441171
C	-4.640649	-2.141607	0.366646
H	-4.831633	-2.762116	-0.520716
H	-5.486015	-2.308567	1.041420
C	-3.344484	-2.592062	1.036457
H	-3.157827	-1.941416	1.905698
H	-3.463837	-3.603026	1.447327
C	-2.133095	-2.550755	0.108425
H	-1.209266	-2.735670	0.667257
H	-2.195649	-3.316320	-0.674969
H	-3.713489	-0.670684	-2.057293
H	0.759340	-3.300585	0.025225
H	-0.197344	1.305655	2.734698
H	0.586814	2.808490	2.188672
H	0.229140	2.586197	-1.772462
H	-0.884408	3.435193	-0.690891
N	2.766978	-1.232725	-0.273832
C	4.082847	-0.640094	-0.258855
H	4.325821	-0.125396	-1.198331
H	4.180071	0.062001	0.573192
H	4.821210	-1.427196	-0.099504

L9 – Octene
Electronic Energy: -1487.40425512
Enthalpy: -1486.864871
Free Energy: -1486.953223

Cr	-1.302864	-0.563611	0.497003
P	0.046578	1.445338	0.167210
N	1.573386	0.757335	-0.261489
C	1.677301	-0.603317	-0.249359

N	0.635263	-1.379750	-0.041831
H	2.395007	1.306568	-0.476769
C	0.408194	2.511671	1.590490
C	-0.301064	2.615303	-1.175183
C	1.152168	-2.754066	-0.002017
C	2.566417	-2.664806	-0.579970
H	3.299276	-3.278870	-0.050767
H	2.601349	-2.931390	-1.646845
H	0.515470	-3.431791	-0.577996
C	-2.269597	-2.498626	0.286021
C	-2.407253	-1.904328	-1.125798
C	-3.840450	-1.674754	-1.584088
C	-4.646273	-0.721726	-0.711652
C	-3.004489	0.639246	0.687134
C	-3.984430	0.636842	-0.478550
H	-3.223600	-2.935970	0.574714
H	-1.850691	-0.945104	-1.324386
H	-4.343721	-2.647522	-1.636151
H	-5.628427	-0.590466	-1.178021
H	-2.693536	1.670889	0.913719
H	-1.503431	-3.274051	0.302716
H	-1.875983	-2.572989	-1.812725
H	-3.814147	-1.289707	-2.611245
H	-4.843616	-1.188259	0.265354
H	-3.525458	0.293205	1.593384
H	-3.490718	0.965990	-1.409063
H	-4.773470	1.381761	-0.300320
C	-1.158777	-0.832296	2.518933
H	-1.569412	0.060859	2.987511
H	-0.141719	-1.094045	2.809472
C	-2.062367	-1.894971	2.206647
H	-3.116914	-1.716791	2.399901
H	-1.751618	-2.912248	2.429013
H	-0.446786	2.077226	-2.114604
H	-0.516132	2.995748	1.919332
H	1.163852	-3.115850	1.036285
H	-1.223083	3.157773	-0.947320
H	0.787621	1.907914	2.417854
H	0.502609	3.346471	-1.301556
H	1.136582	3.290495	1.347267
N	2.863058	-1.242515	-0.409733
C	4.053998	-0.663568	-0.982532
H	3.995395	-0.570681	-2.075697
H	4.253332	0.320300	-0.550929
H	4.908912	-1.295901	-0.736694

L10 – Hexene

Electronic Energy: -1448.10360654
Enthalpy: -1447.595839
Free Energy: -1447.681357

Cr	-1.376530	-0.403530	-0.473600
P	-0.009580	1.523650	0.144070
N	1.586440	0.857770	0.020600
C	1.653560	-0.472420	-0.258150
N	0.571350	-1.195540	-0.463430
H	2.432160	1.352710	0.273430
C	1.038290	-2.539120	-0.845330
C	2.525340	-2.568210	-0.470340
H	2.700490	-3.050700	0.499420
H	3.146370	-3.061690	-1.220170
H	0.895290	-2.684600	-1.923160
H	-2.682630	-1.326720	-0.799330
H	-2.420750	1.575830	-1.923670
H	-3.071850	1.722370	-0.225580
C	-3.436620	-0.206440	-1.164370

C	-2.748060	1.052800	-1.025080
C	-4.570890	-0.559700	-0.210140
H	-4.429760	0.006030	0.723010
H	-5.515180	-0.206340	-0.640390
C	-4.651660	-2.048740	0.116520
H	-4.783590	-2.623310	-0.811850
H	-5.542090	-2.243240	0.722430
C	-3.407880	-2.540450	0.855230
H	-3.307980	-1.959290	1.784470
H	-3.551100	-3.580740	1.174700
C	-2.116400	-2.423250	0.045370
H	-1.243000	-2.567230	0.691980
H	-2.066130	-3.178720	-0.748710
H	-3.605100	-0.541220	-2.193410
H	0.465490	-3.314980	-0.331670
C	-0.261970	1.949030	1.885550
C	-1.073480	1.087010	2.634570
C	0.336040	3.052810	2.507590
C	-1.286960	1.320450	3.988880
H	-1.536290	0.228930	2.138450
C	0.121540	3.282990	3.862020
H	0.956990	3.733920	1.929640
C	-0.688930	2.420420	4.599710
H	-1.921260	0.652770	4.563720
H	0.583120	4.139560	4.343780
H	-0.858080	2.610170	5.655440
C	0.144760	3.090630	-0.746910
C	-0.691240	4.166780	-0.418020
C	1.000170	3.194000	-1.851260
C	-0.653320	5.334380	-1.173480
H	-1.362590	4.096260	0.434910
C	1.035240	4.366420	-2.598970
H	1.642220	2.359820	-2.121650
C	0.210410	5.436720	-2.261390
H	-1.297680	6.166910	-0.908210
H	1.709220	4.442920	-3.446880
H	0.239240	6.350400	-2.847130
N	2.823510	-1.138520	-0.397420
H	3.672260	-0.803780	0.032970

L10 – Octene

Electronic Energy: -1526.70884759
Enthalpy: -1526.140043
Free Energy: -1526.231334

Cr	-1.260447	-0.535404	0.525968
P	0.104856	1.501277	0.169983
N	1.614467	0.786944	-0.293033
C	1.735281	-0.568928	-0.190279
N	0.704468	-1.351026	0.026943
H	2.457427	1.335090	-0.409170
C	1.239119	-2.716139	0.124277
C	2.674160	-2.630635	-0.414811
H	3.389044	-3.214797	0.167768
H	2.739479	-2.947056	-1.463554
H	0.629390	-3.420356	-0.449564
C	-2.226458	-2.420723	0.004159
C	-2.264345	-1.666401	-1.331216
C	-3.659840	-1.362754	-1.856988
C	-4.511904	-0.505175	-0.930672
C	-2.955789	0.666138	0.719980
C	-3.850373	0.806253	-0.504160
H	-3.198325	-2.878826	0.180155
H	-1.702103	-0.694420	-1.369582
H	-4.167511	-2.312977	-2.061244
H	-5.460942	-0.303968	-1.438987

H	-2.630895	1.658938	1.069170
H	-1.463182	-3.198580	-0.012436
H	-1.682949	-2.250459	-2.054272
H	-3.556641	-0.854818	-2.824482
H	-4.775406	-1.079552	-0.029524
H	-3.542325	0.241647	1.549496
H	-3.287875	1.224072	-1.355967
H	-4.639166	1.545097	-0.300047
C	-1.287524	-1.044097	2.513941
H	-1.746406	-0.215360	3.049994
H	-0.291694	-1.334705	2.847165
C	-2.157053	-2.054725	2.008124
H	-3.224273	-1.896315	2.138190
H	-1.858077	-3.093531	2.117506
H	1.222125	-3.046562	1.172182
C	0.525221	2.727589	1.430775
C	0.252610	2.428371	2.771056
C	1.160965	3.933530	1.102090
C	0.613454	3.324062	3.772539
H	-0.245230	1.494614	3.021558
C	1.523613	4.821712	2.107917
H	1.359733	4.178901	0.060957
C	1.249484	4.517537	3.440881
H	0.394634	3.091983	4.810218
H	2.016895	5.754656	1.852441
H	1.529567	5.216797	4.222993
C	-0.413217	2.437341	-1.292682
C	-1.226111	3.569888	-1.150067
C	-0.163073	1.924818	-2.572527
C	-1.765803	4.186078	-2.275414
H	-1.435262	3.971469	-0.161156
C	-0.703853	2.547181	-3.692462
H	0.461726	1.042373	-2.690934
C	-1.506787	3.676723	-3.545314
H	-2.389329	5.066999	-2.157548
H	-0.496099	2.151038	-4.682057
H	-1.929784	4.159628	-4.420913
N	2.934536	-1.197582	-0.288618
H	3.708994	-0.771630	-0.775474

L11 – Hexene

Electronic Energy: -1182.54260868
Enthalpy: -1182.058062
Free Energy: -1182.138045

Cr	-1.349672	-0.427792	-0.457380
P	0.007363	1.490388	0.192538
N	1.597282	0.801086	0.190762
C	1.666853	-0.529716	-0.088971
N	0.593885	-1.218983	-0.431779
H	2.427110	1.289768	0.500319
C	1.041370	-2.608709	-0.620286
C	2.567525	-2.526862	-0.676047
H	3.072109	-3.331658	-0.136173
H	2.949411	-2.510065	-1.707016
H	0.608505	-3.037708	-1.526930
H	-2.662663	-1.341992	-0.786756
H	-2.380424	1.562059	-1.908411
H	-3.034983	1.706606	-0.210421
C	-3.406827	-0.216394	-1.154007
C	-2.710837	1.038780	-1.011157
C	-4.547383	-0.559570	-0.203202
H	-4.404294	0.005460	0.730113
H	-5.487155	-0.197812	-0.636470
C	-4.642536	-2.047316	0.124550
H	-4.777146	-2.621811	-0.803473

H	-5.536249	-2.233121	0.728417
C	-3.405165	-2.548674	0.867092
H	-3.303472	-1.967450	1.796203
H	-3.557950	-3.587434	1.187279
C	-2.109590	-2.443388	0.061652
H	-1.243134	-2.600038	0.713409
H	-2.063645	-3.201724	-0.729917
H	-3.575978	-0.548055	-2.183903
H	0.710077	-3.226248	0.224682
C	-0.354224	1.959686	1.905173
C	-1.152719	1.076572	2.644364
C	0.146936	3.116286	2.515787
C	-1.443941	1.339410	3.978356
H	-1.543951	0.178523	2.157600
C	-0.146812	3.376720	3.849932
H	0.754175	3.814824	1.944540
C	-0.939545	2.491164	4.578777
H	-2.065999	0.653934	4.545617
H	0.241048	4.273985	4.322577
H	-1.168937	2.703091	5.618776
C	0.230013	3.035431	-0.721778
C	-0.705213	4.066630	-0.551549
C	1.237278	3.171839	-1.684517
C	-0.622153	5.219040	-1.325034
H	-1.493088	3.971599	0.192550
C	1.317807	4.331071	-2.450287
H	1.959112	2.372957	-1.834067
C	0.389251	5.353609	-2.273658
H	-1.348124	6.013832	-1.183699
H	2.106694	4.433216	-3.189465
H	0.452397	6.255317	-2.875037
N	2.819717	-1.235337	-0.032976
C	4.143380	-0.657742	-0.032582
H	4.421068	-0.239252	-1.009625
H	4.227956	0.120678	0.729623
H	4.864432	-1.434297	0.226343

L11 – Octene
Electronic Energy: -1261.20282759
Enthalpy: -1260.656473
Free Energy: -1260.739236

Cr	-1.240398	-0.541568	0.602749
P	0.096949	1.476098	0.143867
N	1.589036	0.758847	-0.373988
C	1.722500	-0.594136	-0.226855
N	0.722456	-1.350847	0.168608
H	2.422693	1.312100	-0.528075
C	1.205410	-2.735933	0.097226
C	2.724508	-2.623104	-0.057908
H	3.254965	-2.741573	0.898443
H	3.147222	-3.332420	-0.773709
H	0.758021	-3.244215	-0.768887
C	-2.179952	-2.402820	-0.038063
C	-2.144546	-1.590127	-1.340602
C	-3.509602	-1.251572	-1.922133
C	-4.411365	-0.444544	-0.997919
C	-2.932721	0.676560	0.757187
C	-3.786354	0.855714	-0.490784
H	-3.157168	-2.873905	0.053333
H	-1.563906	-0.626330	-1.311287
H	-4.004686	-2.188286	-2.204988
H	-5.340945	-0.233444	-1.537388
H	-2.614950	1.658347	1.143346
H	-1.410799	-3.175393	-0.044290
H	-1.535622	-2.152470	-2.058348

H	-3.354663	-0.691793	-2.854051
H	-4.704775	-1.060614	-0.134068
H	-3.549969	0.236052	1.555846
H	-3.200615	1.316974	-1.302893
H	-4.593635	1.573780	-0.284171
C	-1.374110	-1.140850	2.555814
H	-1.838454	-0.328351	3.112126
H	-0.404572	-1.475221	2.924180
C	-2.240382	-2.106664	1.955355
H	-3.308727	-1.920958	2.033839
H	-1.982270	-3.157663	2.055411
H	0.915090	-3.296079	0.991510
C	0.556308	2.682367	1.409973
C	0.278639	2.376845	2.747933
C	1.219839	3.875647	1.090648
C	0.664738	3.253670	3.757010
H	-0.244082	1.453090	2.989373
C	1.607247	4.744795	2.103755
H	1.420548	4.125847	0.050889
C	1.329763	4.433886	3.434656
H	0.442857	3.017751	4.793179
H	2.122086	5.668195	1.856095
H	1.629633	5.118337	4.222549
C	-0.469232	2.429641	-1.288520
C	-1.231818	3.590123	-1.101439
C	-0.319198	1.904904	-2.579556
C	-1.818953	4.222183	-2.193844
H	-1.367374	4.000388	-0.103533
C	-0.906384	2.543326	-3.666508
H	0.265298	1.001637	-2.736758
C	-1.657876	3.701272	-3.474942
H	-2.402931	5.124579	-2.040720
H	-0.775875	2.136871	-4.665078
H	-2.118092	4.196375	-4.324589
N	2.865843	-1.250155	-0.543476
C	4.164825	-0.642170	-0.699496
H	4.826886	-1.346822	-1.205370

L12 – Hexene
Electronic Energy: -1221.90180313
Enthalpy: -1221.386789
Free Energy: -1221.467630

Cr	-1.419537	-0.398483	-0.481031
P	-0.021714	1.526064	0.081335
N	1.565051	0.838506	-0.114829
C	1.604330	-0.496709	-0.374874
N	0.505866	-1.196710	-0.563159
H	2.426557	1.314352	0.114293
C	-0.149000	1.824520	1.909719
C	0.100054	3.121981	-0.851535
C	0.930107	-2.594645	-0.745701
C	2.440945	-2.520212	-0.999568
H	3.002576	-3.311924	-0.500712
H	2.679682	-2.543677	-2.070062
H	0.388419	-3.063003	-1.570691
H	-2.696668	-1.394506	-0.665767
H	-2.532390	1.397583	-2.113938
H	-3.195010	1.683044	-0.437222
C	-3.483638	-0.333591	-1.172341
C	-2.834504	0.954279	-1.164791
C	-4.620175	-0.607534	-0.193065
H	-4.532109	0.097890	0.646279
H	-5.569099	-0.371980	-0.688058
C	-4.637632	-2.031848	0.355700
H	-4.737945	-2.749038	-0.471428

H	-5.522296	-2.169573	0.984072
C	-3.377637	-2.344427	1.160850
H	-3.292405	-1.607110	1.973192
H	-3.478663	-3.317672	1.656588
C	-2.097651	-2.325861	0.327144
H	-1.210567	-2.336690	0.972980
H	-2.028864	-3.197150	-0.335598
H	-3.628951	-0.785615	-2.159208
H	0.705332	-3.168799	0.162459
H	0.195808	0.852608	2.295432
H	-0.051394	2.800178	-1.891309
C	-1.612875	1.985683	2.318259
H	-1.696454	2.018293	3.408016
H	-2.054258	2.908629	1.930117
H	-2.227410	1.148536	1.963384
C	0.744217	2.913638	2.488533
H	0.430723	3.911694	2.168801
H	0.691645	2.895429	3.581051
H	1.796090	2.785304	2.215289
C	-1.048292	4.054723	-0.473841
H	-0.929677	4.452751	0.538539
H	-1.066276	4.909838	-1.154412
H	-2.025284	3.568235	-0.535727
C	1.451753	3.823127	-0.766397
H	2.270967	3.195968	-1.127958
H	1.436702	4.714355	-1.400118
H	1.685994	4.155957	0.248229
N	2.757829	-1.208107	-0.427817
H	3.633612	-0.757933	-0.645781

L12 – Octene
Electronic Energy: -1300.45982244
Enthalpy: -1299.885168
Free Energy: -1299.973833

Cr	-1.412355	-0.586959	0.378336
P	-0.209584	1.576755	0.031131
N	1.366346	0.962254	-0.349244
C	1.541821	-0.384591	-0.447172
N	0.553221	-1.236174	-0.306394
H	2.171383	1.558943	-0.487368
C	0.093660	2.649841	1.514543
C	-0.602471	2.606808	-1.461046
C	1.157230	-2.574158	-0.371098
C	2.564249	-2.356519	-0.941303
H	3.324528	-2.976265	-0.462233
H	2.600927	-2.534524	-2.023639
H	0.561683	-3.248844	-0.992668
C	-2.096996	-2.654541	0.337225
C	-2.471199	-2.157400	-1.066553
C	-3.963783	-2.203000	-1.363999
C	-4.821589	-1.379522	-0.412962
C	-3.269265	0.318527	0.706474
C	-4.390813	0.081766	-0.296974
H	-2.938980	-3.203776	0.753986
H	-2.125344	-1.120896	-1.344934
H	-4.283604	-3.251524	-1.344685
H	-5.859864	-1.443038	-0.755554
H	-3.086495	1.398555	0.806613
H	-1.228693	-3.311063	0.297657
H	-1.902457	-2.750270	-1.792040
H	-4.124130	-1.852656	-2.391325
H	-4.813154	-1.833469	0.589263
H	-3.605029	-0.015704	1.700295
H	-4.108397	0.447627	-1.298537
H	-5.267321	0.683911	-0.015921

C	-1.022689	-0.733806	2.389953
H	-1.523963	0.108551	2.865122
H	0.047024	-0.818187	2.579197
C	-1.770476	-1.935719	2.218131
H	-2.813650	-1.917005	2.521527
H	-1.277169	-2.881552	2.424551
H	-0.395518	1.883330	-2.263982
H	1.199936	-3.007562	0.638905
H	0.122601	1.912004	2.328310
C	-2.085379	2.957193	-1.528784
H	-2.309570	3.426570	-2.491412
H	-2.721485	2.071821	-1.435192
H	-2.382388	3.664177	-0.749070
C	0.284007	3.826253	-1.672936
H	1.352594	3.592769	-1.620848
H	0.096934	4.251914	-2.663912
H	0.070705	4.611870	-0.941570
C	1.417791	3.403060	1.525104
H	1.470100	4.170844	0.748824
H	1.534411	3.911638	2.487109
H	2.277907	2.736207	1.415944
C	-1.091276	3.578876	1.756455
H	-2.051547	3.053001	1.741519
H	-0.994670	4.054109	2.736909
H	-1.131499	4.380625	1.012372
N	2.766600	-0.941163	-0.638914
H	3.507530	-0.424517	-1.089154

L13 – Hexene
Electronic Energy: -1261.16770566
Enthalpy: -1260.624953
Free Energy: -1260.709213

Cr	-1.409638	-0.418801	-0.500509
P	-0.022789	1.494191	0.160513
N	1.558330	0.784848	0.057256
C	1.610910	-0.537474	-0.252935
N	0.518852	-1.219070	-0.549516
H	2.421150	1.281008	0.233903
C	-0.210819	1.856110	1.970432
C	0.158425	3.065708	-0.802982
C	0.944803	-2.611913	-0.759351
C	2.469266	-2.542885	-0.885778
H	2.990876	-3.348065	-0.362794
H	2.803835	-2.538064	-1.932949
H	0.469808	-3.034041	-1.648185
H	-2.705150	-1.398388	-0.680907
H	-2.531548	1.418420	-2.074937
H	-3.175698	1.680417	-0.387904
C	-3.484622	-0.323987	-1.160265
C	-2.826571	0.960595	-1.129611
C	-4.619509	-0.609834	-0.183450
H	-4.521456	0.072725	0.673373
H	-5.569440	-0.353581	-0.667417
C	-4.649282	-2.047498	0.327635
H	-4.759856	-2.739453	-0.519661
H	-5.533441	-2.193558	0.955999
C	-3.389218	-2.398744	1.116612
H	-3.294852	-1.690607	1.953504
H	-3.500753	-3.387573	1.579634
C	-2.110899	-2.363792	0.281220
H	-1.223620	-2.393806	0.925119
H	-2.048595	-3.219925	-0.401898
H	-3.642549	-0.751636	-2.156095
H	0.643773	-3.227855	0.098336
H	0.078081	0.886696	2.403327

H	0.031240	2.725031	-1.839690
C	-1.677176	2.090859	2.324951
H	-1.797066	2.137340	3.411419
H	-2.061650	3.029501	1.915080
H	-2.316154	1.278626	1.956757
C	0.710556	2.923697	2.543851
H	0.446289	3.926202	2.193377
H	0.632214	2.933853	3.635601
H	1.762559	2.745096	2.298828
C	-0.978402	4.029855	-0.476729
H	-0.868878	4.459392	0.524004
H	-0.971572	4.861559	-1.187141
H	-1.963861	3.559594	-0.536122
C	1.519432	3.743328	-0.695123
H	2.337846	3.096414	-1.024477
H	1.537322	4.624100	-1.344300
H	1.735406	4.088972	0.319470
N	2.759245	-1.250268	-0.263386
C	4.087690	-0.688444	-0.276748
H	4.354570	-0.254655	-1.249948
H	4.190637	0.074655	0.499388
H	4.805882	-1.476040	-0.043768

L13 – Octene

Electronic Energy: -1339.77507028
Enthalpy: -1339.170719
Free Energy: -1339.258477

Cr	-1.365738	-0.479597	0.509137
P	-0.004778	1.548639	0.176097
N	1.516880	0.823259	-0.245591
C	1.592743	-0.536749	-0.310228
N	0.535846	-1.303292	-0.154931
H	2.328228	1.361985	-0.516023
C	0.469764	2.649721	1.587514
C	-0.338663	2.606176	-1.306547
C	1.034121	-2.684813	-0.182405
C	2.443385	-2.587216	-0.770730
H	3.166805	-3.254298	-0.295476
H	2.458302	-2.778793	-1.854220
H	0.382825	-3.326839	-0.782370
C	-2.292486	-2.453346	0.341650
C	-2.516312	-1.855546	-1.058203
C	-3.978049	-1.680155	-1.445830
C	-4.772974	-0.770942	-0.518607
C	-3.097197	0.655990	0.783117
C	-4.152786	0.611036	-0.314672
H	-3.221821	-2.909781	0.677366
H	-2.011634	-0.871875	-1.272279
H	-4.443756	-2.671525	-1.490287
H	-5.784725	-0.676960	-0.925627
H	-2.807854	1.698893	0.973748
H	-1.512888	-3.213846	0.312067
H	-1.988619	-2.495413	-1.774885
H	-4.017036	-1.279437	-2.466716
H	-4.895245	-1.251566	0.463703
H	-3.544514	0.306248	1.726842
H	-3.737571	0.966072	-1.274200
H	-4.956069	1.323344	-0.078211
C	-1.081435	-0.780865	2.511358
H	-1.484762	0.081710	3.038339
H	-0.041236	-1.022130	2.728367
C	-1.980366	-1.862516	2.245367
H	-3.022560	-1.707413	2.511306
H	-1.634910	-2.873691	2.441547
H	0.589632	3.161974	-1.506847

H	1.052736	-3.094410	0.838341
H	1.022504	1.952299	2.233444
C	-0.644739	1.694100	-2.490681
H	-0.726613	2.277547	-3.411826
H	0.123926	0.930291	-2.645397
H	-1.605239	1.183712	-2.343206
C	-1.472680	3.597408	-1.067646
H	-1.234212	4.338573	-0.301037
H	-1.684473	4.143780	-1.991005
H	-2.396814	3.088115	-0.773360
C	1.399462	3.786755	1.180103
H	0.892847	4.516078	0.540176
H	1.745682	4.323730	2.067595
H	2.292663	3.438330	0.651052
C	-0.746052	3.144292	2.366805
H	-1.390493	2.321593	2.687466
H	-0.415987	3.678150	3.262112
H	-1.359768	3.838353	1.785897
N	2.771101	-1.187374	-0.500039
C	3.970404	-0.586339	-1.033713
H	3.904748	-0.386293	-2.112301
H	4.200105	0.343362	-0.506687
H	4.811103	-1.259909	-0.861582

L14 – Hexene

Electronic Energy: -2314.54067193
Enthalpy: -2314.213870
Free Energy: -2314.305179

Cr	-1.459226	-0.371911	-0.519405
P	-0.071581	1.562416	0.107128
N	1.512944	0.856455	-0.042393
C	1.564943	-0.446251	-0.427437
N	0.477074	-1.129673	-0.711887
H	2.372785	1.323510	0.209683
C	-0.298968	1.829409	1.954761
C	0.142920	3.147988	-0.870546
C	0.916582	-2.503716	-1.006571
C	2.431095	-2.396858	-1.219394
H	2.988036	-3.231646	-0.790443
H	2.692031	-2.311182	-2.281654
H	0.395357	-2.902063	-1.879960
H	-2.732307	-1.393731	-0.624613
H	-2.731737	1.362938	-2.112186
H	-3.234803	1.714827	-0.395053
C	-3.581018	-0.329501	-1.028948
C	-2.938363	0.957458	-1.121805
C	-4.596586	-0.575034	0.081179
H	-4.406175	0.146655	0.889872
H	-5.595913	-0.339657	-0.302651
C	-4.560951	-1.986411	0.659992
H	-4.778540	-2.719526	-0.129664
H	-5.357400	-2.095835	1.401810
C	-3.210358	-2.304877	1.297281
H	-3.000483	-1.546271	2.068463
H	-3.260137	-3.261268	1.832420
C	-2.059627	-2.337608	0.294419
H	-1.093804	-2.409470	0.806940
H	-2.133411	-3.198932	-0.380773
H	-3.839252	-0.802186	-1.982339
H	0.680704	-3.157336	-0.156667
C	-1.786640	2.110650	2.195632
H	-1.963033	2.231479	3.269550
H	-2.139398	3.020493	1.701865
H	-2.411052	1.276379	1.851045
C	0.559998	2.937859	2.555328

H	0.279468	3.928407	2.186966
H	0.428467	2.950118	3.642755
H	1.627968	2.787963	2.364319
C	-1.035018	4.081527	-0.591776
H	-1.014964	4.482654	0.425999
H	-0.986888	4.935580	-1.275062
H	-2.000082	3.591131	-0.752865
C	1.463666	3.864273	-0.582203
H	2.331023	3.250748	-0.845758
H	1.520358	4.760465	-1.208885
H	1.564583	4.191133	0.454387
C	0.131238	2.715999	-2.341651
H	-0.816229	2.248865	-2.623552
H	0.274751	3.593415	-2.980708
H	0.939312	2.011195	-2.564588
C	0.050754	0.489819	2.614239
H	-0.529793	-0.340873	2.190838
H	1.111600	0.241503	2.521200
H	-0.187893	0.540725	3.681487
N	2.724317	-1.147129	-0.511571
H	3.603108	-0.675293	-0.661172

L14 – Octene

Electronic Energy: -2393.15092006
Enthalpy: -2392.761872
Free Energy: -2392.858325

Cr	-1.318346	-0.463099	0.520519
P	0.055028	1.583181	-0.052207
N	1.494425	0.797905	-0.633168
C	1.606853	-0.551565	-0.466483
N	0.595486	-1.309821	-0.121874
H	2.344776	1.313685	-0.815994
C	0.670576	2.640311	1.377705
C	-0.445922	2.598544	-1.551307
C	1.131096	-2.672317	0.005314
C	2.521789	-2.629622	-0.644865
H	3.276273	-3.187545	-0.087079
H	2.504175	-3.005344	-1.675605
H	0.477726	-3.400697	-0.484269
C	-2.264969	-2.422899	0.266384
C	-2.488157	-1.778577	-1.103622
C	-3.951928	-1.574079	-1.472244
C	-4.750892	-0.744129	-0.476059
C	-3.051820	0.666829	0.824482
C	-4.171861	0.643262	-0.207766
H	-3.189754	-2.892756	0.595352
H	-1.969437	-0.794809	-1.273570
H	-4.413625	-2.561575	-1.588735
H	-5.773957	-0.657964	-0.856035
H	-2.740720	1.705093	1.007189
H	-1.475547	-3.172434	0.226114
H	-1.969245	-2.393162	-1.849182
H	-3.999035	-1.098453	-2.460372
H	-4.838336	-1.283862	0.478971
H	-3.454599	0.317679	1.788127
H	-3.842091	1.083682	-1.162921
H	-4.986073	1.299505	0.131628
C	-1.074774	-0.837099	2.531625
H	-1.461455	0.030091	3.064077
H	-0.045895	-1.112910	2.758767
C	-1.987341	-1.886466	2.224282
H	-3.035631	-1.721935	2.457855
H	-1.664365	-2.912061	2.377944
H	1.190207	-2.947608	1.067613
C	-1.079292	1.591887	-2.518528

H	-1.318308	2.089474	-3.464352
H	-0.403778	0.758529	-2.745227
H	-2.013276	1.186038	-2.115833
C	-1.490589	3.637740	-1.143437
H	-1.066721	4.436234	-0.527663
H	-1.900827	4.108625	-2.042930
H	-2.330085	3.190049	-0.600056
C	1.498540	3.854053	0.962666
H	0.910312	4.599330	0.420989
H	1.888066	4.343560	1.861908
H	2.364698	3.585420	0.347941
C	-0.555085	3.084944	2.182022
H	-1.123461	2.226850	2.553835
H	-0.225178	3.666830	3.048972
H	-1.237409	3.717002	1.606808
C	1.527890	1.717579	2.250758
H	1.000437	0.795584	2.513689
H	2.470001	1.443282	1.767138
H	1.774799	2.235466	3.183015
C	0.735522	3.268599	-2.254475
H	1.467386	2.535736	-2.607719
H	0.364586	3.794110	-3.140807
H	1.247219	4.007688	-1.635925
N	2.799274	-1.192796	-0.617580
H	3.512528	-0.810296	-1.219800

L15 – Hexene
Electronic Energy: -2314.54067193
Enthalpy: -2314.213870
Free Energy: -2314.305179

Cr	-1.503792	-0.614730	-0.486369
P	-0.190646	1.293345	0.189801
N	1.436402	0.755908	0.133270
C	1.580533	-0.515295	-0.311812
N	0.562458	-1.313958	-0.520347
H	2.263591	1.332853	0.254107
C	-0.352645	1.999306	1.924612
C	-0.054067	2.887769	-0.798740
C	1.128310	-2.548402	-0.979590
C	2.628450	-2.286668	-1.121629
H	3.236124	-2.979930	-0.542902
H	2.947818	-2.259390	-2.163428
H	-2.837167	-1.498049	-0.869165
H	-2.554426	1.304954	-2.005784
H	-3.086263	1.624796	-0.287856
C	-3.602228	-0.350212	-1.033648
C	-2.846753	0.876860	-1.045597
C	-4.572640	-0.584728	0.117684
H	-4.288854	0.078992	0.947487
H	-5.571662	-0.264277	-0.199159
C	-4.605065	-2.020979	0.629208
H	-4.972829	-2.693557	-0.157941
H	-5.322592	-2.092426	1.451747
C	-3.229099	-2.491091	1.089856
H	-2.840946	-1.782807	1.843331
H	-3.307587	-3.451856	1.614589
C	-2.231546	-2.622166	-0.053795
H	-1.249039	-2.947488	0.293399
H	-2.564815	-3.342405	-0.809471
H	-3.950332	-0.704254	-2.009074
F	-0.238736	0.995105	2.801665
F	-1.561784	2.556201	2.053566
F	0.581727	2.913411	2.198708
F	-0.033909	2.589746	-2.103762
F	1.071301	3.551724	-0.505100

F	-1.104477	3.669691	-0.543432
F	0.887558	-3.548591	-0.090572
F	0.552749	-2.932318	-2.144303
O	2.796925	-0.955216	-0.565365

L15 – Octene
Electronic Energy: -2393.15092006
Enthalpy: -2392.761872
Free Energy: -2392.858325

Cr	-1.402652	-0.571874	0.327746
P	0.051845	1.372023	0.061125
N	1.560433	0.738790	-0.439153
C	1.643263	-0.614559	-0.486817
N	0.627535	-1.396505	-0.244663
H	2.390740	1.288618	-0.638922
C	0.532503	2.421721	1.547479
C	-0.216529	2.736482	-1.204895
C	1.128559	-2.726390	-0.340010
C	2.601120	-2.591969	-0.733998
H	3.275664	-3.007453	0.013812
H	2.808506	-3.005817	-1.720262
C	-2.333110	-2.504430	0.354819
C	-2.622541	-2.017694	-1.074168
C	-4.097993	-1.829137	-1.390725
C	-4.802418	-0.804339	-0.512923
C	-3.027872	0.706257	0.546187
C	-4.128032	0.567035	-0.494612
H	-3.236108	-2.951455	0.764919
H	-2.102895	-1.070862	-1.404075
H	-4.591819	-2.803623	-1.303000
H	-5.835009	-0.711587	-0.863627
H	-2.680020	1.749078	0.580914
H	-1.527040	-3.237870	0.362558
H	-2.148368	-2.734345	-1.753067
H	-4.874036	-1.181371	0.518442
H	-3.427854	0.494689	1.548388
H	-3.747229	0.804909	-1.500759
H	-4.891089	1.332455	-0.296054
C	-1.058894	-0.673484	2.347539
H	-1.406530	0.264762	2.777715
H	-0.026392	-0.942446	2.566888
C	-2.003063	-1.734307	2.207097
H	-3.037932	-1.518175	2.460077
H	-1.685468	-2.735474	2.482824
F	-0.565726	2.939110	2.102275
F	1.365548	3.416038	1.215334
F	-0.956662	3.707604	-0.663316
F	-0.865455	2.232835	-2.262217
F	0.943987	3.252098	-1.627576
F	1.145933	1.637092	2.441741
H	-4.189295	-1.532062	-2.442348
F	0.970813	-3.377680	0.845991
F	0.417026	-3.445373	-1.249108
O	2.811160	-1.155730	-0.785690

L16 – Hexene
Electronic Energy: -1838.99833525
Enthalpy: -1838.702395
Free Energy: -1838.783263

Cr	-1.503792	-0.614730	-0.486369
P	-0.190646	1.293345	0.189801
N	1.436402	0.755908	0.133270
C	1.580533	-0.515295	-0.311812
N	0.562458	-1.313958	-0.520347

H	2.263591	1.332853	0.254107
C	-0.352645	1.999306	1.924612
C	-0.054067	2.887769	-0.798740
C	1.128310	-2.548402	-0.979590
C	2.628450	-2.286668	-1.121629
H	3.236124	-2.979930	-0.542902
H	2.947818	-2.259390	-2.163428
H	-2.837167	-1.498049	-0.869165
H	-2.554426	1.304954	-2.005784
H	-3.086263	1.624796	-0.287856
C	-3.602228	-0.350212	-1.033648
C	-2.846753	0.876860	-1.045597
C	-4.572640	-0.584728	0.117684
H	-4.288854	0.078992	0.947487
H	-5.571662	-0.264277	-0.199159
C	-4.605065	-2.020979	0.629208
H	-4.972829	-2.693557	-0.157941
H	-5.322592	-2.092426	1.451747
C	-3.229099	-2.491091	1.089856
H	-2.840946	-1.782807	1.843331
H	-3.307587	-3.451856	1.614589
C	-2.231546	-2.622166	-0.053795
H	-1.249039	-2.947488	0.293399
H	-2.564815	-3.342405	-0.809471
H	-3.950332	-0.704254	-2.009074
F	-0.238736	0.995105	2.801665
F	-1.561784	2.556201	2.053566
F	0.581727	2.913411	2.198708
F	-0.033909	2.589746	-2.103762
F	1.071301	3.551724	-0.505100
F	-1.104477	3.669691	-0.543432
F	0.887558	-3.548591	-0.090572
F	0.552749	-2.932318	-2.144303
O	2.796925	-0.955216	-0.565365

L16 – Octene

Electronic Energy: -1917.61192843
Enthalpy: -1917.254814
Free Energy: -1917.340690

Cr	-1.402652	-0.571874	0.327746
P	0.051845	1.372023	0.061125
N	1.560433	0.738790	-0.439153
C	1.643263	-0.614559	-0.486817
N	0.627535	-1.396505	-0.244663
H	2.390740	1.288618	-0.638922
C	0.532503	2.421721	1.547479
C	-0.216529	2.736482	-1.204895
C	1.128559	-2.726390	-0.340010
C	2.601120	-2.591969	-0.733998
H	3.275664	-3.007453	0.013812
H	2.808506	-3.005817	-1.720262
C	-2.333110	-2.504430	0.354819
C	-2.622541	-2.017694	-1.074168
C	-4.097993	-1.829137	-1.390725
C	-4.802418	-0.804339	-0.512923
C	-3.027872	0.706257	0.546187
C	-4.128032	0.567035	-0.494612
H	-3.236108	-2.951455	0.764919
H	-2.102895	-1.070862	-1.404075
H	-4.591819	-2.803623	-1.303000
H	-5.835009	-0.711587	-0.863627
H	-2.680020	1.749078	0.580914
H	-1.527040	-3.237870	0.362558
H	-2.148368	-2.734345	-1.753067
H	-4.874036	-1.181371	0.518442

H	-3.427854	0.494689	1.548388
H	-3.747229	0.804909	-1.500759
H	-4.891089	1.332455	-0.296054
C	-1.058894	-0.673484	2.347539
H	-1.406530	0.264762	2.777715
H	-0.026392	-0.942446	2.566888
C	-2.003063	-1.734307	2.207097
H	-3.037932	-1.518175	2.460077
H	-1.685468	-2.735474	2.482824
F	-0.565726	2.939110	2.102275
F	1.365548	3.416038	1.215334
F	-0.956662	3.707604	-0.663316
F	-0.865455	2.232835	-2.262217
F	0.943987	3.252098	-1.627576
F	1.145933	1.637092	2.441741
H	-4.189295	-1.532062	-2.442348
F	0.970813	-3.377680	0.845991
F	0.417026	-3.445373	-1.249108
O	2.811160	-1.155730	-0.785690

L17 – Hexene

Electronic Energy: -1640.54002895
Enthalpy: -1640.229370
Free Energy: -1640.308608

Cr	-1.503792	-0.614730	-0.486369
P	-0.190646	1.293345	0.189801
N	1.436402	0.755908	0.133270
C	1.580533	-0.515295	-0.311812
N	0.562458	-1.313958	-0.520347
H	2.263591	1.332853	0.254107
C	-0.352645	1.999306	1.924612
C	-0.054067	2.887769	-0.798740
C	1.128310	-2.548402	-0.979590
C	2.628450	-2.286668	-1.121629
H	3.236124	-2.979930	-0.542902
H	2.947818	-2.259390	-2.163428
H	-2.837167	-1.498049	-0.869165
H	-2.554426	1.304954	-2.005784
H	-3.086263	1.624796	-0.287856
C	-3.602228	-0.350212	-1.033648
C	-2.846753	0.876860	-1.045597
C	-4.572640	-0.584728	0.117684
H	-4.288854	0.078992	0.947487
H	-5.571662	-0.264277	-0.199159
C	-4.605065	-2.020979	0.629208
H	-4.972829	-2.693557	-0.157941
H	-5.322592	-2.092426	1.451747
C	-3.229099	-2.491091	1.089856
H	-2.840946	-1.782807	1.843331
H	-3.307587	-3.451856	1.614589
C	-2.231546	-2.622166	-0.053795
H	-1.249039	-2.947488	0.293399
H	-2.564815	-3.342405	-0.809471
H	-3.950332	-0.704254	-2.009074
F	-0.238736	0.995105	2.801665
F	-1.561784	2.556201	2.053566
F	0.581727	2.913411	2.198708
F	-0.033909	2.589746	-2.103762
F	1.071301	3.551724	-0.505100
F	-1.104477	3.669691	-0.543432
F	0.887558	-3.548591	-0.090572
F	0.552749	-2.932318	-2.144303
O	2.796925	-0.955216	-0.565365

L17 – Octene

Electronic Energy: -1719.14890505
Enthalpy: -1718.777185
Free Energy: -1718.859955

Cr	-1.402652	-0.571874	0.327746
P	0.051845	1.372023	0.061125
N	1.560433	0.738790	-0.439153
C	1.643263	-0.614559	-0.486817
N	0.627535	-1.396505	-0.244663
H	2.390740	1.288618	-0.638922
C	0.532503	2.421721	1.547479
C	-0.216529	2.736482	-1.204895
C	1.128559	-2.726390	-0.340010
C	2.601120	-2.591969	-0.733998
H	3.275664	-3.007453	0.013812
H	2.808506	-3.005817	-1.720262
C	-2.333110	-2.504430	0.354819
C	-2.622541	-2.017694	-1.074168
C	-4.097993	-1.829137	-1.390725
C	-4.802418	-0.804339	-0.512923
C	-3.027872	0.706257	0.546187
C	-4.128032	0.567035	-0.494612
H	-3.236108	-2.951455	0.764919
H	-2.102895	-1.070862	-1.404075
H	-4.591819	-2.803623	-1.303000
H	-5.835009	-0.711587	-0.863627
H	-2.680020	1.749078	0.580914
H	-1.527040	-3.237870	0.362558
H	-2.148368	-2.734345	-1.753067
H	-4.874036	-1.181371	0.518442
H	-3.427854	0.494689	1.548388
H	-3.747229	0.804909	-1.500759
H	-4.891089	1.332455	-0.296054
C	-1.058894	-0.673484	2.347539
H	-1.406530	0.264762	2.777715
H	-0.026392	-0.942446	2.566888
C	-2.003063	-1.734307	2.207097
H	-3.037932	-1.518175	2.460077
H	-1.685468	-2.735474	2.482824
F	-0.565726	2.939110	2.102275
F	1.365548	3.416038	1.215334
F	-0.956662	3.707604	-0.663316
F	-0.865455	2.232835	-2.262217
F	0.943987	3.252098	-1.627576
F	1.145933	1.637092	2.441741
H	-4.189295	-1.532062	-2.442348
F	0.970813	-3.377680	0.845991
F	0.417026	-3.445373	-1.249108
O	2.811160	-1.155730	-0.785690

L18 – Hexene
Electronic Energy: -1719.21336817
Enthalpy: -1718.845235
Free Energy: -1718.926955

Cr	-1.493468	-0.569222	-0.519192
P	-0.172881	1.328337	0.161203
N	1.432189	0.766058	0.088747
C	1.544008	-0.524310	-0.342756
N	0.514349	-1.277124	-0.608010
H	2.273141	1.318800	0.216747
C	-0.335737	1.976583	1.916638
C	-0.036224	2.954549	-0.769154
C	1.063484	-2.594098	-0.968602
C	2.569377	-2.346318	-1.083021
H	3.193173	-3.039138	-0.519836

H	2.927883	-2.282530	-2.112445
H	0.626635	-2.949822	-1.904541
H	-2.808505	-1.488570	-0.861320
H	-2.585952	1.327532	-2.032326
H	-3.104311	1.645474	-0.309684
C	-3.600576	-0.338749	-1.045347
C	-2.865881	0.898819	-1.068807
C	-4.560008	-0.593480	0.110416
H	-4.272450	0.059116	0.947877
H	-5.563815	-0.273674	-0.192157
C	-4.582200	-2.038448	0.598841
H	-4.937133	-2.700579	-0.203265
H	-5.306847	-2.131173	1.413099
C	-3.207903	-2.505121	1.069955
H	-2.842394	-1.809508	1.844896
H	-3.286477	-3.478984	1.569857
C	-2.184636	-2.591596	-0.058024
H	-1.197036	-2.874504	0.319401
H	-2.470396	-3.333908	-0.812585
H	-3.943740	-0.709734	-2.016259
H	0.823655	-3.324970	-0.188709
F	-0.152540	0.951139	2.758785
F	-1.568616	2.466358	2.093531
F	0.556813	2.928400	2.204076
F	-0.073489	2.711860	-2.085251
F	1.112653	3.585823	-0.493910
F	-1.059954	3.747337	-0.440201
O	2.756329	-1.017854	-0.489721

L18 – Octene
Electronic Energy: -1797.82273933
Enthalpy: -1797.392583
Free Energy: -1797.479071

Cr	-1.387525	-0.557351	0.324637
P	0.061071	1.379388	0.077200
N	1.550983	0.731686	-0.416722
C	1.616379	-0.634782	-0.464018
N	0.601963	-1.409183	-0.236935
H	2.386021	1.267681	-0.627963
C	0.524546	2.438808	1.560937
C	-0.215863	2.737327	-1.191933
C	1.126239	-2.779071	-0.291727
C	2.562784	-2.612375	-0.800656
H	3.324147	-3.083508	-0.179695
H	2.699899	-2.915422	-1.840571
H	0.523809	-3.400598	-0.960633
C	-2.310253	-2.495784	0.343579
C	-2.603688	-2.008807	-1.084737
C	-4.082518	-1.835625	-1.396732
C	-4.792438	-0.818099	-0.514640
C	-3.027755	0.711739	0.535207
C	-4.132455	0.560561	-0.500335
H	-3.207819	-2.958423	0.748678
H	-2.097581	-1.054174	-1.409604
H	-4.566808	-2.814969	-1.308357
H	-5.828095	-0.737474	-0.859501
H	-2.688886	1.757592	0.562544
H	-1.495411	-3.221133	0.354175
H	-2.128635	-2.717050	-1.772649
H	-4.853920	-1.196309	0.517061
H	-3.427515	0.507146	1.539374
H	-3.758370	0.799569	-1.508738
H	-4.903960	1.317391	-0.301438
C	-1.065049	-0.660387	2.351155
H	-1.419379	0.278830	2.773034

H	-0.033197	-0.923264	2.580364
C	-2.005604	-1.721728	2.200068
H	-3.044243	-1.506357	2.437790
H	-1.694136	-2.722968	2.483621
H	1.086617	-3.229835	0.707734
F	-0.579412	2.955699	2.107783
F	1.355678	3.436542	1.231580
F	-0.959944	3.710487	-0.657369
F	-0.864417	2.226533	-2.247684
F	0.941292	3.256876	-1.620223
F	1.134783	1.662654	2.465737
H	-4.180376	-1.537546	-2.447449
O	2.793013	-1.167582	-0.744839

L19 – Hexene

Electronic Energy: -1123.83918276
Enthalpy: -1123.428899
Free Energy: -1123.502920

Cr	-1.519256	-0.792345	-0.415522
P	-0.309872	1.239145	0.176466
N	1.328220	0.639298	0.269404
C	1.518683	-0.618564	-0.160146
N	0.540666	-1.470711	-0.370560
H	2.151021	1.215388	0.407695
C	-0.620815	1.945252	1.818663
C	-0.143137	2.694352	-0.892183
C	1.152849	-2.603169	-1.052488
C	2.665003	-2.385532	-0.861279
H	3.080533	-3.015199	-0.072924
H	3.254083	-2.500104	-1.771430
H	-2.863365	-1.740163	-0.476771
H	-2.437267	0.573923	-2.443057
H	-3.044737	1.431694	-0.951743
C	-3.594113	-0.667610	-1.056784
C	-2.791549	0.477011	-1.414330
H	0.621626	3.383936	-0.524155
H	-1.629142	2.370597	1.827372
C	-4.603178	-0.495815	0.072927
H	-4.327936	0.406841	0.639681
H	-5.589346	-0.292545	-0.360646
C	-4.677550	-1.668417	1.045612
H	-5.031492	-2.569432	0.525684
H	-5.422452	-1.448854	1.816498
C	-3.324168	-1.957594	1.688950
H	-2.944494	-1.028043	2.150016
H	-3.437880	-2.667346	2.518488
C	-2.307154	-2.494051	0.691207
H	-1.323990	-2.657752	1.146323
H	-2.629220	-3.450069	0.267719
H	-3.929609	-1.306030	-1.879903
H	-0.576865	1.164643	2.581356
H	0.090573	2.737582	2.067736
H	0.102519	2.391124	-1.912226
H	-1.096953	3.227995	-0.919256
C	0.750768	-2.510670	-2.534246
F	1.119439	-3.585864	-3.229667
F	1.328282	-1.425933	-3.082833
F	-0.584694	-2.353478	-2.664765
C	0.753849	-3.958348	-0.454816
F	0.834769	-3.914536	0.882044
F	1.598646	-4.906984	-0.890246
F	-0.487946	-4.319871	-0.797709
O	2.757635	-1.007150	-0.431226

L19 – Octene

Electronic Energy: -1202.44873689
Enthalpy: -1201.977036
Free Energy: -1202.053909

24	-1.388499	-0.670889	0.459580
15	-0.025587	1.318553	0.069139
7	1.544190	0.670130	-0.282217
6	1.685865	-0.667714	-0.302977
7	0.717449	-1.527341	-0.104459
1	2.368877	1.224408	-0.480942
6	0.279634	2.445532	1.455330
6	-0.345212	2.429009	-1.329556
6	1.352155	-2.837752	-0.150475
6	2.795179	-2.563206	-0.623186
1	3.563711	-3.010642	0.007229
1	2.963707	-2.855656	-1.661668
6	-2.704674	-2.411568	0.580062
6	-2.772162	-2.022639	-0.907938
6	-4.160917	-1.655568	-1.413312
6	-4.810946	-0.480561	-0.697145
6	-2.963159	0.716165	0.588833
6	-3.925835	0.759408	-0.589223
1	-3.717413	-2.545332	0.954182
1	-2.098739	-1.184042	-1.251559
1	-4.799981	-2.542176	-1.333765
1	-5.740078	-0.237337	-1.222627
1	-2.551291	1.719002	0.775568
1	-2.145592	-3.336118	0.699882
1	-2.352548	-2.853268	-1.482808
1	-4.082759	-1.431290	-2.484454
1	-5.115073	-0.780768	0.316231
1	-3.515564	0.458977	1.503484
1	-3.385963	0.911170	-1.539556
1	-4.573949	1.641781	-0.489551
6	-1.159350	-0.681387	2.491295
1	-1.420525	0.308652	2.861910
1	-0.165169	-1.040790	2.757958
6	-2.213488	-1.641971	2.385928
1	-3.212327	-1.295459	2.634051
1	-2.015986	-2.655655	2.717845
1	-0.459160	1.856346	-2.252579
1	-0.663196	2.916795	1.747963
1	-1.275879	2.974200	-1.147828
1	0.665290	1.889661	2.312408
1	0.457906	3.160215	-1.457115
1	0.988032	3.234473	1.187871
6	0.659363	-3.771611	-1.152951
6	1.360620	-3.442830	1.260753
8	2.911669	-1.128648	-0.537271
9	1.449049	-4.817380	-1.437651
9	-0.505679	-4.251689	-0.690872
9	0.410525	-3.114722	-2.295550
9	2.098686	-2.663565	2.071559
9	1.892292	-4.671275	1.259544
9	0.128717	-3.516740	1.784931

L20 – Hexene
Electronic Energy: -1243.67209290
Enthalpy: -1243.334873
Free Energy: -1243.406199

Cr	-1.479920	-0.596193	-0.372494
P	-0.176788	1.371399	0.313954
N	1.429121	0.733170	0.165305
C	1.524985	-0.532370	-0.305445
N	0.507289	-1.329511	-0.475114

H	2.278293	1.284047	0.199361
C	-0.271658	1.938542	2.036441
C	-0.091604	2.918699	-0.630003
C	1.052903	-2.618036	-0.992233
C	2.517841	-2.243448	-1.302405
H	3.251119	-2.951932	-0.914114
H	2.702500	-2.075292	-2.368468
H	-2.760538	-1.596156	-0.573033
H	-2.387904	1.031954	-2.228463
H	-3.150547	1.553152	-0.654160
C	-3.506207	-0.526305	-1.174907
C	-2.791521	0.722268	-1.263021
H	0.705058	3.572573	-0.263768
H	-1.241566	2.414950	2.205691
C	-4.676217	-0.638217	-0.204214
H	-4.596222	0.180104	0.525796
H	-5.607494	-0.462879	-0.755519
C	-4.745919	-1.961139	0.554043
H	-4.881473	-2.793005	-0.151924
H	-5.630187	-1.962061	1.198528
C	-3.490992	-2.202724	1.389642
H	-3.332752	-1.332478	2.047048
H	-3.639187	-3.056640	2.062716
C	-2.244551	-2.428384	0.540592
H	-1.337323	-2.449281	1.156978
H	-2.292240	-3.377663	-0.006255
H	-3.649287	-1.066630	-2.116364
H	-0.185983	1.089115	2.717275
H	0.514138	2.663226	2.266987
H	0.072155	2.710957	-1.689371
H	-1.041763	3.450533	-0.531106
C	0.296376	-3.028937	-2.242937
H	0.727848	-3.932591	-2.684124
H	-0.750034	-3.249889	-2.006095
H	0.320771	-2.236781	-2.997952
C	0.988421	-3.701180	0.076490
H	-0.042109	-3.972235	0.312623
H	1.493997	-4.605135	-0.277000
H	1.481784	-3.378206	0.998289
O	2.736130	-0.974632	-0.624151

L20 – Octene

Electronic Energy: -1322.28492113
Enthalpy: -1321.886371
Free Energy: -1321.963125

24	-1.349132	-0.594081	0.418205
15	0.000603	1.404481	0.053105
7	1.547448	0.719028	-0.280733
6	1.641257	-0.634947	-0.311486
7	0.646365	-1.459792	-0.166404
1	2.393295	1.245930	-0.460484
6	0.301345	2.530805	1.441682
6	-0.319249	2.517263	-1.344676
6	1.237811	-2.828284	-0.175302
6	2.693368	-2.560471	-0.615789
1	3.445557	-3.041697	0.012513
1	2.877068	-2.820854	-1.663323
6	-2.458114	-2.460490	0.469341
6	-2.669013	-1.987616	-0.978902
6	-4.119080	-1.717597	-1.356466
6	-4.806549	-0.646307	-0.521987
6	-2.984192	0.703789	0.644355
6	-4.045469	0.676362	-0.446234
1	-3.411114	-2.796565	0.873309
1	-2.085549	-1.079393	-1.307653

1	-4.672431	-2.661125	-1.284159
1	-5.806255	-0.485354	-0.938578
1	-2.611210	1.730996	0.774556
1	-1.744084	-3.283649	0.503876
1	-2.227172	-2.743537	-1.637893
1	-4.147990	-1.427148	-2.414039
1	-4.969551	-1.016297	0.501387
1	-3.447651	0.442339	1.607118
1	-3.604981	0.904728	-1.431647
1	-4.769432	1.484418	-0.268266
6	-1.069802	-0.674226	2.447410
1	-1.400930	0.278342	2.857515
1	-0.045320	-0.961292	2.683538
6	-2.045447	-1.708054	2.311315
1	-3.069601	-1.454453	2.570449
1	-1.767996	-2.718803	2.599328
1	-0.434620	1.943229	-2.266778
1	-0.641119	3.004156	1.732413
1	-1.251361	3.060111	-1.162130
1	0.681795	1.971996	2.299190
1	0.482970	3.248915	-1.475756
1	1.014185	3.317725	1.179865
6	0.544476	-3.732407	-1.181494
1	1.107959	-4.663363	-1.300916
1	-0.461610	-4.008384	-0.856010
1	0.475627	-3.251146	-2.161456
6	1.176366	-3.409363	1.231013
1	0.142761	-3.446007	1.589496
1	1.573435	-4.429008	1.250626
1	1.757580	-2.806775	1.935897
8	2.866600	-1.126572	-0.489763

L21 – Hexene

Electronic Energy: -1045.21121333
Enthalpy: -1044.858765
Free Energy: -1044.926509

Cr	-1.483930	-0.547327	-0.423917
P	-0.138678	1.415968	0.221492
N	1.484345	0.795943	0.027667
C	1.581981	-0.482148	-0.361166
N	0.543649	-1.279894	-0.485375
H	2.335368	1.345022	0.069460
C	-0.155221	2.050164	1.920603
C	-0.099071	2.918061	-0.793742
C	1.069666	-2.547715	-0.875311
C	2.558949	-2.318889	-1.127654
H	3.192345	-2.997982	-0.559596
H	2.805896	-2.351356	-2.189441
H	-2.787511	-1.476543	-0.782561
H	-2.562791	1.365595	-1.928278
H	-3.146219	1.614626	-0.216976
C	-3.574101	-0.353101	-1.033275
C	-2.856991	0.897586	-0.987664
H	0.705417	3.592564	-0.487721
H	-1.123479	2.520919	2.113922
C	-4.608114	-0.642915	0.047279
H	-4.378711	-0.015715	0.921538
H	-5.591070	-0.316060	-0.311666
C	-4.653392	-2.102326	0.488315
H	-4.924826	-2.741595	-0.363521
H	-5.446360	-2.230927	1.231398
C	-3.317848	-2.562494	1.065478
H	-3.050624	-1.898406	1.904205
H	-3.421328	-3.561302	1.509007
C	-2.184850	-2.575942	0.046196

H	-1.232291	-2.820971	0.520078
H	-2.353160	-3.321124	-0.740073
H	-3.850144	-0.711193	-2.030243
H	-0.026681	1.231688	2.631462
H	0.628198	2.795664	2.081999
H	0.027851	2.662580	-1.847804
H	-1.049698	3.446716	-0.683324
F	0.421910	-3.026728	-1.967279
F	0.882366	-3.477395	0.105701
O	2.781575	-0.970081	-0.648421

L21 – Octene
Electronic Energy: -1123.81934959
Enthalpy: -1123.406015
Free Energy: -1123.480051

Cr	-1.358205	-0.558854	0.397424
P	0.027378	1.454809	0.062628
N	1.568765	0.751544	-0.355933
C	1.645537	-0.588119	-0.414195
N	0.629082	-1.385693	-0.197922
H	2.415599	1.277704	-0.539561
C	0.418678	2.520989	1.473609
C	-0.294772	2.610324	-1.296513
C	1.127056	-2.707105	-0.326316
C	2.609854	-2.568446	-0.673872
H	3.258583	-2.996823	0.090019
H	2.847540	-2.976456	-1.656003
C	-2.304824	-2.504102	0.297329
C	-2.556858	-1.939624	-1.109532
C	-4.021720	-1.730384	-1.463820
C	-4.762151	-0.758628	-0.555129
C	-3.028488	0.644334	0.684452
C	-4.087348	0.605524	-0.407867
H	-3.227131	-2.945135	0.669766
H	-2.034157	-0.973965	-1.366787
H	-4.519753	-2.706795	-1.452391
H	-5.777604	-0.638334	-0.946295
H	-2.692995	1.679485	0.850600
H	-1.523823	-3.262750	0.272714
H	-2.063096	-2.614098	-1.816905
H	-4.076156	-1.372017	-2.499356
H	-4.880812	-1.202024	0.444883
H	-3.475442	0.325164	1.637975
H	-3.662574	0.912906	-1.378590
H	-4.860529	1.355938	-0.189580
C	-1.052906	-0.774786	2.408799
H	-1.439388	0.121989	2.890957
H	-0.012993	-1.019497	2.624192
C	-1.959475	-1.857659	2.192524
H	-2.998701	-1.693030	2.464001
H	-1.609723	-2.864580	2.400392
H	-0.415001	2.063432	-2.234393
H	-0.497034	3.020633	1.803076
H	-1.229973	3.140259	-1.092267
H	0.795127	1.920226	2.304188
H	0.501861	3.350866	-1.409408
H	1.155000	3.287397	1.216698
F	0.440766	-3.396618	-1.283665
F	0.934383	-3.412043	0.826873
O	2.821015	-1.136608	-0.704460

L22 – Hexene
Electronic Energy: -2102.65434220
Enthalpy: -2102.172830
Free Energy: -2102.270423

Cr	-1.471487	-0.515517	-0.454090
P	-0.152928	1.445012	0.208541
N	1.456694	0.805803	0.100760
C	1.548743	-0.480317	-0.300243
N	0.513232	-1.237356	-0.548739
H	2.314474	1.334080	0.201776
C	-0.250077	2.113418	1.893320
C	-0.077344	2.932899	-0.827638
C	1.048651	-2.567576	-0.867530
C	2.554725	-2.336068	-0.998718
H	3.175666	-3.026867	-0.428925
H	2.903305	-2.302612	-2.033665
H	0.605927	-2.953756	-1.789108
H	-2.751493	-1.479866	-0.793294
H	-2.597187	1.388386	-1.939639
H	-3.172716	1.616755	-0.222812
C	-3.565796	-0.355097	-1.047930
C	-2.875916	0.909839	-0.999855
H	0.082048	2.659920	-1.872926
H	-1.214398	2.612703	2.024537
C	-4.588688	-0.681890	0.032235
H	-4.359366	-0.076031	0.921532
H	-5.578530	-0.356852	-0.309547
C	-4.615920	-2.154084	0.432708
H	-4.869950	-2.771925	-0.440387
H	-5.414425	-2.316767	1.163085
C	-3.281051	-2.614003	1.013611
H	-3.037142	-1.973465	1.876361
H	-3.376723	-3.628747	1.421067
C	-2.130297	-2.567303	0.011999
H	-1.176169	-2.772395	0.508351
H	-2.249775	-3.317695	-0.779466
H	-3.836072	-0.716009	-2.045582
H	0.808439	-3.274795	-0.065091
H	-0.181176	1.308415	2.627562
H	0.542556	2.842295	2.083599
H	-1.027894	3.468321	-0.755674
H	0.721732	3.607750	-0.508148
O	2.759229	-1.002738	-0.436488

L22 – Octene

Electronic Energy: -2181.25835744
Enthalpy: -2180.714551
Free Energy: -2180.816368

Cr	-1.338949	-0.543173	0.406447
P	0.055820	1.444668	0.045264
N	1.561008	0.707139	-0.387781
C	1.603955	-0.646655	-0.425135
N	0.580691	-1.420078	-0.205797
H	2.413378	1.207107	-0.608490
C	0.470939	2.526693	1.439003
C	-0.288520	2.589727	-1.318757
C	1.093757	-2.791865	-0.240103
C	2.527109	-2.642150	-0.758635
H	3.285711	-3.136431	-0.151842
H	2.647269	-2.940622	-1.802860
H	0.486298	-3.422779	-0.896523
C	-2.300991	-2.483686	0.292691
C	-2.562306	-1.906342	-1.107180
C	-4.029510	-1.687212	-1.446723
C	-4.755841	-0.715744	-0.526213
C	-3.005385	0.674496	0.703619
C	-4.073992	0.645304	-0.380339
H	-3.218132	-2.937206	0.663479

H	-2.035541	-0.942473	-1.357602
H	-4.533561	-2.660728	-1.436565
H	-5.774941	-0.590951	-0.906645
H	-2.665427	1.708370	0.869074
H	-1.515257	-3.239265	0.258301
H	-2.084504	-2.576048	-1.831040
H	-4.090936	-1.322195	-2.479544
H	-4.865948	-1.162965	0.473168
H	-3.451524	0.359955	1.659574
H	-3.654217	0.952016	-1.353592
H	-4.843473	1.398092	-0.156899
C	-1.040685	-0.776951	2.419055
H	-1.418384	0.124610	2.898813
H	-0.003463	-1.030609	2.636729
C	-1.960690	-1.845676	2.193318
H	-2.999602	-1.666887	2.457304
H	-1.631535	-2.859478	2.404208
H	0.516020	3.316553	-1.461512
H	-0.433351	3.047114	1.767643
H	1.058039	-3.231603	0.765422
H	-0.436939	2.032595	-2.246631
H	0.844610	1.931872	2.275124
H	-1.210829	3.135904	-1.099728
H	1.219642	3.275132	1.165303
O	2.780149	-1.207108	-0.689834

L23 – Hexene
Electronic Energy: -1507.27921015
Enthalpy: -1506.755113
Free Energy: -1506.842511

Cr	-1.243599	-0.721592	-0.484488
P	-0.202625	1.426006	0.020189
N	1.472889	0.947864	0.218360
C	1.762824	-0.318234	-0.118725
N	0.844366	-1.242993	-0.279485
H	2.241742	1.597737	0.338430
C	1.535084	-2.400840	-0.824250
C	3.030018	-2.059163	-0.670005
H	3.501966	-2.601178	0.151618
H	3.614348	-2.192966	-1.581516
H	-2.507582	-1.763306	-0.379733
H	-2.159401	0.134284	-2.780428
H	-2.875460	1.221515	-1.496891
C	-3.284840	-0.900150	-1.218339
C	-2.552455	0.214889	-1.764957
C	-4.371760	-0.613758	-0.189345
H	-4.198569	0.392298	0.221237
H	-5.340148	-0.570133	-0.701963
C	-4.425252	-1.607710	0.967383
H	-4.658576	-2.612679	0.587931
H	-5.247584	-1.336755	1.636723
C	-3.111792	-1.651997	1.745647
H	-2.862878	-0.631941	2.080565
H	-3.236944	-2.240726	2.663961
C	-1.965568	-2.225537	0.923796
H	-1.004775	-2.183751	1.451853
H	-2.144782	-3.275381	0.671414
H	-3.509448	-1.720283	-1.907296
C	-0.776201	1.756005	1.707299
C	-1.846917	2.637405	1.914371
C	-0.299627	0.982240	2.774636
C	-2.413387	2.757427	3.179789
H	-2.232501	3.233220	1.089574
C	-0.867225	1.113762	4.037536
H	0.518758	0.282660	2.618833

C	-1.924515	1.998593	4.240804
H	-3.236183	3.448272	3.336060
H	-0.484943	0.521690	4.863474
H	-2.368449	2.095472	5.226780
C	-0.112838	3.019768	-0.818313
C	0.212808	4.197012	-0.128329
C	-0.350419	3.060450	-2.198641
C	0.301266	5.399403	-0.819716
H	0.384893	4.171029	0.945408
C	-0.260045	4.268255	-2.882526
H	-0.612334	2.147604	-2.729115
C	0.064133	5.434458	-2.193295
H	0.550960	6.311028	-0.285595
H	-0.449664	4.300128	-3.950780
H	0.128385	6.377675	-2.727343
C	1.121164	-2.525992	-2.298746
F	1.547405	-3.659613	-2.853678
F	1.623437	-1.492154	-2.996092
F	-0.225538	-2.470013	-2.420702
C	1.217461	-3.689232	-0.054033
F	2.099487	-4.646350	-0.383155
F	-0.010968	-4.148816	-0.320351
F	1.315562	-3.468763	1.263822
O	3.028860	-0.650901	-0.335047

L23 – Octene

Electronic Energy: -1585.88789151
Enthalpy: -1585.302804
Free Energy: -1585.394968

Cr	-1.367600	-0.588449	0.546214
P	-0.006102	1.404026	0.105124
N	1.456740	0.688437	-0.506209
C	1.665618	-0.632177	-0.339528
N	0.776935	-1.502071	0.075923
H	2.250624	1.230171	-0.829148
C	1.513705	-2.759776	0.193235
C	2.857588	-2.492110	-0.515349
H	3.732991	-2.814468	0.048332
H	2.897822	-2.920264	-1.519345
C	-2.558445	-2.345106	0.010468
C	-2.446718	-1.583797	-1.325881
C	-3.769686	-1.118257	-1.917832
C	-4.583039	-0.192018	-1.026466
C	-2.971014	0.743930	0.707400
C	-3.805475	1.024441	-0.531825
H	-3.591508	-2.665667	0.130809
H	-1.756212	-0.694562	-1.350363
H	-4.358753	-2.007030	-2.172754
H	-5.468525	0.124832	-1.587307
H	-2.574633	1.680868	1.129420
H	-1.919463	-3.221799	-0.020950
H	-1.923914	-2.249270	-2.020143
H	-3.556149	-0.609581	-2.867238
H	-4.966944	-0.748089	-0.158107
H	-3.617242	0.319496	1.489462
H	-3.184193	1.417264	-1.351732
H	-4.516796	1.832267	-0.305480
C	-1.563528	-1.052229	2.510315
H	-2.012299	-0.208258	3.031396
H	-0.619468	-1.403278	2.919720
C	-2.466349	-2.026549	1.956159
H	-3.524643	-1.822593	2.095196
H	-2.213427	-3.074475	2.100091
C	0.521811	2.570373	1.377308
C	0.259402	2.257374	2.716718

C	1.227554	3.739635	1.057157
C	0.698473	3.106662	3.727490
H	-0.289851	1.350147	2.959250
C	1.667581	4.579836	2.072481
H	1.421164	3.993366	0.017120
C	1.402552	4.263701	3.404933
H	0.490290	2.865096	4.765056
H	2.215584	5.484013	1.825800
H	1.745475	4.925501	4.194541
C	-0.589244	2.381591	-1.299375
C	-1.272713	3.586094	-1.091261
C	-0.530300	1.832726	-2.588247
C	-1.871916	4.239186	-2.164731
H	-1.340855	4.012489	-0.093425
C	-1.127261	2.493418	-3.655872
H	-0.008408	0.893157	-2.758002
C	-1.800366	3.695825	-3.444471
H	-2.396191	5.175063	-1.997647
H	-1.067194	2.070055	-4.653942
H	-2.269530	4.208357	-4.278636
C	0.812931	-3.940508	-0.494868
F	-0.178733	-4.461693	0.244460
F	1.696615	-4.923305	-0.727891
F	0.300009	-3.555912	-1.673520
C	1.765932	-3.079804	1.676059
F	2.479329	-4.208670	1.801284
F	0.632186	-3.224865	2.372743
F	2.466181	-2.076127	2.232249
O	2.892203	-1.058495	-0.635328

L24 – Hexene
Electronic Energy: -1627.11124666
Enthalpy: -1626.660712
Free Energy: -1626.747876

Cr	-1.392028	-0.505871	-0.459395
P	-0.065163	1.461879	0.177618
N	1.533508	0.798190	0.089458
C	1.618809	-0.506307	-0.261004
N	0.591043	-1.291237	-0.429193
H	2.395038	1.319917	0.195875
C	1.135588	-2.631412	-0.797008
C	2.617825	-2.306545	-1.073744
H	3.321348	-3.000814	-0.612128
H	2.844400	-2.212255	-2.141089
H	-2.710075	-1.448370	-0.676110
H	-2.202895	1.156255	-2.331720
H	-2.983754	1.686730	-0.771157
C	-3.392854	-0.379985	-1.320552
C	-2.643011	0.848826	-1.382244
C	-4.601013	-0.475138	-0.396972
H	-4.508593	0.299957	0.378324
H	-5.500529	-0.223390	-0.971009
C	-4.760445	-1.835202	0.277122
H	-4.862367	-2.619021	-0.487114
H	-5.690574	-1.850170	0.853488
C	-3.580356	-2.159783	1.190772
H	-3.492530	-1.358153	1.940784
H	-3.787102	-3.073738	1.761933
C	-2.252948	-2.310339	0.449120
H	-1.409356	-2.312564	1.150308
H	-2.213110	-3.250792	-0.113751
H	-3.512814	-0.916215	-2.267734
C	-0.387453	1.875372	1.908152
C	-1.366881	1.125100	2.570683
C	0.308118	2.875571	2.600662

C	-1.650357	1.365470	3.911138
H	-1.907054	0.350006	2.020742
C	0.027015	3.109074	3.941506
H	1.058120	3.472728	2.086010
C	-0.950312	2.356831	4.594246
H	-2.414437	0.784551	4.418812
H	0.566252	3.882540	4.479729
H	-1.168913	2.548818	5.640403
C	0.130348	3.039355	-0.686497
C	-0.648915	4.143084	-0.314636
C	0.970464	3.131722	-1.803993
C	-0.569268	5.327482	-1.040322
H	-1.308283	4.081000	0.547989
C	1.050241	4.321644	-2.519117
H	1.569926	2.277419	-2.108696
C	0.281476	5.419414	-2.138952
H	-1.169955	6.181244	-0.742088
H	1.714719	4.390974	-3.374987
H	0.345436	6.346917	-2.699568
C	0.428801	-3.155113	-2.034134
H	0.863085	-4.104561	-2.361694
H	-0.631128	-3.334666	-1.826087
H	0.502161	-2.443068	-2.861917
C	1.010776	-3.602767	0.370274
H	-0.032333	-3.832463	0.595190
H	1.509904	-4.545823	0.126521
H	1.477359	-3.199200	1.273953
O	2.834832	-0.999713	-0.471397

L24 – Octene
Electronic Energy: -1705.72408541
Enthalpy: -1705.212181
Free Energy: -1705.304586

Cr	-1.288054	-0.570129	0.643040
P	0.051680	1.448131	0.088408
N	1.536971	0.722043	-0.428934
C	1.682846	-0.611560	-0.214529
N	0.731630	-1.422002	0.144511
H	2.384332	1.251183	-0.599334
C	1.328795	-2.788717	0.116508
C	2.835616	-2.478822	0.051245
H	3.322287	-2.514186	1.032019
H	3.392271	-3.099059	-0.653354
C	-2.402664	-2.369902	0.116716
C	-2.359860	-1.612061	-1.216666
C	-3.716658	-1.183982	-1.758655
C	-4.527370	-0.292469	-0.828166
C	-2.903678	0.743354	0.845248
C	-3.790514	0.965296	-0.370790
H	-3.408087	-2.758006	0.270103
H	-1.697015	-0.702599	-1.250969
H	-4.287563	-2.088068	-2.001399
H	-5.452996	-0.021733	-1.346998
H	-2.510644	1.704720	1.212243
H	-1.695428	-3.199675	0.108832
H	-1.831301	-2.249816	-1.935651
H	-3.553803	-0.658875	-2.708989
H	-4.842553	-0.864194	0.058028
H	-3.513531	0.344077	1.669721
H	-3.209179	1.371868	-1.213799
H	-4.533202	1.743268	-0.140446
C	-1.385657	-1.086652	2.626457
H	-1.770104	-0.222934	3.166288
H	-0.424952	-1.471467	2.967448
C	-2.340602	-2.011384	2.104874

H	-3.389250	-1.751490	2.223664
H	-2.148194	-3.073986	2.229879
C	0.534247	2.678575	1.321825
C	0.284620	2.402886	2.671894
C	1.206747	3.855962	0.963871
C	0.705305	3.294057	3.654123
H	-0.240941	1.490396	2.946265
C	1.629010	4.739138	1.950521
H	1.390399	4.082218	-0.084210
C	1.378465	4.458290	3.293270
H	0.505933	3.080320	4.699635
H	2.152303	5.648975	1.672764
H	1.707549	5.152765	4.060382
C	-0.522436	2.363292	-1.362547
C	-1.253632	3.548266	-1.210279
C	-0.397922	1.785300	-2.633509
C	-1.835513	4.153709	-2.320462
H	-1.368278	3.997935	-0.226746
C	-0.980648	2.396924	-3.737848
H	0.164792	0.862092	-2.757681
C	-1.700755	3.580284	-3.582070
H	-2.394517	5.076147	-2.196785
H	-0.870200	1.951049	-4.721818
H	-2.156480	4.055337	-4.445429
C	0.879561	-3.523183	-1.141708
H	1.363352	-4.502903	-1.205628
H	-0.200479	-3.691662	-1.145645
H	1.139666	-2.960018	-2.043825
C	0.972571	-3.565060	1.370304
H	-0.103893	-3.753232	1.424169
H	1.475468	-4.537013	1.377088
H	1.271393	-3.021230	2.270910
O	2.904411	-1.106763	-0.418470

L25 – Hexene

Electronic Energy: -1428.64491161
Enthalpy: -1428.180721
Free Energy: -1428.264710

Cr	-1.493514	-0.452109	-0.598744
P	0.000748	1.419843	-0.085399
N	1.572955	0.654204	-0.233449
C	1.556727	-0.636281	-0.592645
N	0.448905	-1.341648	-0.644210
H	2.461168	1.142174	-0.217147
C	0.819042	-2.644217	-1.079567
C	2.333792	-2.593843	-1.290020
H	2.865724	-3.286599	-0.638644
H	2.616168	-2.746273	-2.331482
H	-2.870986	-1.336602	-0.574029
H	-2.520562	0.990409	-2.556956
H	-2.940604	1.828098	-0.989139
C	-3.598522	-0.245446	-1.118845
C	-2.783670	0.879044	-1.503985
C	-4.549603	-0.096528	0.061274
H	-4.197697	0.739096	0.685602
H	-5.535744	0.199300	-0.315942
C	-4.659827	-1.345987	0.930283
H	-5.043141	-2.184077	0.331107
H	-5.397378	-1.174109	1.720288
C	-3.318061	-1.732081	1.547977
H	-2.937335	-0.872979	2.124511
H	-3.457814	-2.537109	2.281039
C	-2.276620	-2.159515	0.519405
H	-1.293711	-2.304347	0.978774
H	-2.542495	-3.104814	0.031652

H	-3.984581	-0.862850	-1.935932
C	-0.229230	1.644273	1.697603
C	0.273732	0.695512	2.597550
C	-1.080746	2.657858	2.159944
C	-0.049097	0.778697	3.947815
H	0.921704	-0.102915	2.243204
C	-1.404564	2.728622	3.511136
H	-1.479119	3.395535	1.466082
C	-0.889077	1.792295	4.404734
H	0.355202	0.050081	4.643835
H	-2.056208	3.520759	3.866764
H	-1.142087	1.852226	5.458763
C	0.258092	3.060835	-0.784717
C	-0.222268	3.326704	-2.073491
C	0.951874	4.053535	-0.076594
C	-0.007552	4.574216	-2.649985
H	-0.766578	2.557703	-2.616156
C	1.164922	5.296004	-0.661694
H	1.312045	3.856352	0.930582
C	0.684666	5.555592	-1.944846
H	-0.384987	4.781480	-3.646281
H	1.701208	6.065301	-0.114878
H	0.847387	6.530100	-2.395199
F	0.144338	-2.973702	-2.217300
F	0.473566	-3.590233	-0.166282
O	2.692882	-1.239980	-0.913884

L25 – Octene

Electronic Energy: -1507.25840605
Enthalpy: -1506.731653
Free Energy: -1506.819868

Cr	-1.304722	-0.535570	0.517297
P	0.089808	1.505464	0.163077
N	1.620112	0.787307	-0.293994
C	1.718646	-0.550847	-0.251551
N	0.701674	-1.350094	-0.043439
H	2.472755	1.315442	-0.442983
C	1.217052	-2.669307	-0.096342
C	2.725959	-2.526158	-0.296833
H	3.291748	-2.865738	0.571263
H	3.076213	-3.017350	-1.204061
C	-2.258230	-2.431159	0.034608
C	-2.319258	-1.687048	-1.306178
C	-3.719068	-1.372164	-1.812577
C	-4.555874	-0.503447	-0.882943
C	-2.978651	0.666143	0.745765
C	-3.882639	0.805856	-0.469711
H	-3.227014	-2.886120	0.233332
H	-1.738848	-0.725187	-1.369666
H	-4.236358	-2.319465	-2.004731
H	-5.507810	-0.297635	-1.383489
H	-2.637265	1.654834	1.089979
H	-1.491374	-3.203532	0.008267
H	-1.756816	-2.289304	-2.028339
H	-3.624347	-0.871913	-2.784864
H	-4.815451	-1.070314	0.023854
H	-3.551496	0.239896	1.583144
H	-3.327737	1.220339	-1.328132
H	-4.663885	1.549571	-0.255703
C	-1.260202	-1.033407	2.503191
H	-1.706494	-0.208540	3.055683
H	-0.251862	-1.319936	2.800654
C	-2.138026	-2.054746	2.031511
H	-3.201703	-1.905011	2.196313
H	-1.821973	-3.088499	2.133221

C	0.526156	2.719742	1.424356
C	0.225504	2.427652	2.760547
C	1.194517	3.909981	1.101855
C	0.592342	3.316308	3.765869
H	-0.298447	1.506555	3.004616
C	1.562973	4.789820	2.112365
H	1.414099	4.148680	0.063490
C	1.261871	4.493327	3.441512
H	0.353126	3.091152	4.800429
H	2.082413	5.710209	1.863883
H	1.547889	5.186371	4.226909
C	-0.404517	2.434613	-1.308799
C	-1.171857	3.599675	-1.177556
C	-0.189563	1.885310	-2.580357
C	-1.701818	4.212776	-2.309228
H	-1.353028	4.028552	-0.194734
C	-0.718708	2.506886	-3.705802
H	0.397348	0.975462	-2.689990
C	-1.476352	3.669063	-3.571048
H	-2.289744	5.119057	-2.202207
H	-0.538186	2.084240	-4.689531
H	-1.890988	4.150710	-4.451224
F	0.638997	-3.375433	-1.115614
F	0.906945	-3.361984	1.035439
O	2.916578	-1.098268	-0.438732

L26 – Hexene
Electronic Energy: -1431.47123925
Enthalpy: -1430.928166
Free Energy: -1431.015073

Cr	-1.444599	-0.517409	-0.821241
P	-0.154159	1.422880	0.317680
N	1.401644	0.643411	0.294193
C	1.498449	-0.574719	-0.282660
N	0.513187	-1.187335	-0.881427
H	2.247780	1.046138	0.679646
C	1.012787	-2.515134	-1.253217
C	2.522494	-2.397847	-1.046529
H	2.975000	-3.216396	-0.487957
H	3.078445	-2.236136	-1.973617
H	0.749883	-2.754120	-2.285894
H	-2.303906	-1.612557	-1.703379
H	-2.831140	1.574672	-1.585358
H	-3.482181	1.035323	0.060539
C	-3.743925	-0.367367	-1.549283
C	-3.211584	0.766708	-0.960253
C	-4.724328	-1.283835	-0.863107
H	-5.423711	-0.638166	-0.316243
H	-5.311966	-1.795477	-1.630978
C	-4.181469	-2.328912	0.111967
H	-3.626661	-3.092035	-0.449245
H	-5.046778	-2.835460	0.552300
C	-3.285426	-1.775681	1.218213
H	-3.685322	-0.811173	1.569817
H	-3.354907	-2.445163	2.088616
C	-1.830343	-1.646074	0.823144
H	-1.212587	-1.220224	1.628485
H	-1.411272	-2.628777	0.564180
H	-3.707713	-0.426065	-2.634931
H	0.557725	-3.275406	-0.606687
C	-0.399922	1.939574	2.032027
C	-1.494119	1.434015	2.743179
C	0.481723	2.835429	2.654368
C	-1.699311	1.812064	4.067343
H	-2.182043	0.745387	2.256015

C	0.277739	3.200810	3.978771
H	1.316770	3.256221	2.097653
C	-0.811234	2.688470	4.684343
H	-2.550405	1.420595	4.615662
H	0.963948	3.890433	4.460576
H	-0.968850	2.979303	5.718562
C	0.149892	2.962620	-0.595494
C	-0.584204	4.113371	-0.277648
C	1.005202	2.974727	-1.705023
C	-0.448383	5.262179	-1.050785
H	-1.251568	4.116322	0.581243
C	1.141109	4.129372	-2.468617
H	1.578995	2.087714	-1.963091
C	0.413831	5.272526	-2.144383
H	-1.013462	6.152659	-0.792790
H	1.818553	4.136408	-3.317224
H	0.521451	6.172319	-2.742230
O	2.674810	-1.185674	-0.241997

L26 – Octene
Electronic Energy: -1510.08156423
Enthalpy: -1509.478103
Free Energy: -1509.569162

Cr	-1.272684	-0.536559	0.590174
P	0.055490	1.503684	0.121781
N	1.548616	0.784044	-0.397615
C	1.687398	-0.553723	-0.221109
N	0.723229	-1.348289	0.139443
H	2.388401	1.314594	-0.596737
C	1.284527	-2.700899	0.139358
C	2.780343	-2.490181	-0.123313
H	3.409082	-2.662410	0.753226
H	3.176046	-3.055491	-0.967586
H	0.812838	-3.308062	-0.643480
C	-2.182305	-2.411505	-0.049071
C	-2.170822	-1.592720	-1.349013
C	-3.544677	-1.271005	-1.919424
C	-4.450014	-0.477018	-0.987477
C	-2.976540	0.648352	0.766357
C	-3.835506	0.826859	-0.476955
H	-3.148866	-2.903382	0.045388
H	-1.604387	-0.620141	-1.322638
H	-4.029626	-2.213416	-2.200398
H	-5.383852	-0.272372	-1.521742
H	-2.663286	1.627600	1.161383
H	-1.396584	-3.167232	-0.065422
H	-1.559042	-2.144273	-2.072797
H	-3.403468	-0.708042	-2.851442
H	-4.733466	-1.099488	-0.124971
H	-3.583161	0.191095	1.563287
H	-3.258539	1.299798	-1.288584
H	-4.648387	1.535222	-0.260308
C	-1.376481	-1.146179	2.538810
H	-1.850884	-0.346177	3.104553
H	-0.398189	-1.464544	2.898835
C	-2.230115	-2.127059	1.942273
H	-3.300934	-1.963313	2.033724
H	-1.949571	-3.172761	2.036777
H	1.097751	-3.198404	1.097106
C	0.522136	2.708833	1.382849
C	0.253586	2.400937	2.722371
C	1.195923	3.895513	1.060141
C	0.658173	3.270377	3.730334
H	-0.273574	1.480375	2.966628
C	1.601211	4.756971	2.072585

H	1.393929	4.144280	0.019678
C	1.332750	4.444325	3.404975
H	0.445480	3.032576	4.767940
H	2.125575	5.674474	1.823450
H	1.649195	5.121906	4.192277
C	-0.508681	2.435746	-1.322057
C	-1.240415	3.619192	-1.160876
C	-0.381418	1.868908	-2.597996
C	-1.820129	4.233937	-2.267219
H	-1.356397	4.061105	-0.174075
C	-0.961289	2.490319	-3.698259
H	0.182305	0.947545	-2.730273
C	-1.682312	3.671932	-3.533534
H	-2.379614	5.155101	-2.136576
H	-0.848454	2.053319	-4.685928
H	-2.136558	4.154342	-4.393560
O	2.888028	-1.074681	-0.457970

L27 – Hexene
Electronic Energy: -1604.64499344
Enthalpy: -1604.310436
Free Energy: -1604.389140

24	-1.489024	-0.441262	-0.487393
15	-0.032754	1.481721	0.100190
7	1.539082	0.782517	-0.188879
6	1.550750	-0.521874	-0.516790
7	0.475404	-1.259491	-0.600162
1	2.427009	1.267429	-0.152867
6	-0.040804	1.776812	1.930615
6	0.045992	3.074821	-0.844674
6	0.931784	-2.621982	-0.845670
6	2.399538	-2.413533	-1.280554
1	3.133257	-3.110386	-0.879105
1	2.471238	-2.385574	-2.370673
1	-2.812114	-1.382307	-0.682487
1	-2.578167	1.446166	-2.019078
1	-3.240289	1.657703	-0.332712
6	-3.558003	-0.318251	-1.170464
6	-2.887910	0.959327	-1.093477
6	-4.726812	-0.602189	-0.232326
1	-4.661391	0.089937	0.619746
1	-5.658545	-0.355686	-0.754560
6	-4.765623	-2.032391	0.296929
1	-4.846568	-2.738626	-0.542060
1	-5.666423	-2.172900	0.902548
6	-3.523320	-2.358016	1.123640
1	-3.453404	-1.629930	1.945984
1	-3.642294	-3.336404	1.607359
6	-2.229682	-2.345453	0.316634
1	-1.347744	-2.381273	0.966225
1	-2.154954	-3.201052	-0.363863
1	-3.690834	-0.723412	-2.179146
1	0.296073	0.793787	2.292863
1	-0.178178	2.752615	-1.870628
6	-1.471438	1.983274	2.422590
1	-1.491286	1.986957	3.516614
1	-1.892259	2.935284	2.085313
1	-2.138698	1.181201	2.082176
6	0.919006	2.836692	2.451940
1	0.611673	3.845088	2.158178
1	0.940973	2.811304	3.546079
1	1.944726	2.679280	2.100045
6	-1.065646	4.017204	-0.390692
1	-0.871186	4.417438	0.609263
1	-1.123779	4.867968	-1.075366

1	-2.049133	3.539829	-0.378760
6	1.401917	3.770285	-0.851233
1	2.189792	3.160016	-1.301687
1	1.333341	4.682274	-1.452125
1	1.721634	4.070118	0.150421
8	0.130196	-3.128566	-1.868501
6	0.235744	-4.529080	-2.073128
1	-0.096774	-5.091760	-1.193983
1	-0.418338	-4.764438	-2.912737
1	1.259477	-4.834304	-2.335472
8	0.760942	-3.336193	0.352820
6	1.737505	-4.289547	0.743234
1	2.643839	-3.812185	1.138100
1	1.280636	-4.870979	1.545091
1	2.015767	-4.978653	-0.063185
8	2.724928	-1.093811	-0.774505

L27 – Octene
Electronic Energy: -1683.25388002
Enthalpy: -1682.857992
Free Energy: -1682.940903

Cr	-1.468180	-0.601393	0.495154
P	-0.223369	1.525332	-0.012075
N	1.329153	0.870791	-0.446812
C	1.500790	-0.465137	-0.399629
N	0.579154	-1.309561	-0.041761
H	2.121931	1.429362	-0.737716
C	0.170853	2.633995	1.422717
C	-0.640643	2.516487	-1.522875
C	1.163501	-2.627835	-0.128718
C	2.648795	-2.361645	-0.482517
H	3.347862	-2.572873	0.329086
H	2.968640	-2.877056	-1.390004
C	-2.203968	-2.643620	0.547049
C	-2.581620	-2.195337	-0.870144
C	-4.076932	-2.210673	-1.153030
C	-4.904310	-1.329577	-0.227781
C	-3.290335	0.369722	0.793899
C	-4.434507	0.122662	-0.179204
H	-3.051249	-3.158929	0.995281
H	-2.203783	-1.182416	-1.198817
H	-4.423395	-3.248990	-1.088717
H	-5.948487	-1.379743	-0.554378
H	-3.070231	1.446537	0.842692
H	-1.335529	-3.299342	0.521299
H	-2.024107	-2.834495	-1.563218
H	-4.239790	-1.898001	-2.192150
H	-4.892668	-1.741189	0.792473
H	-3.616000	0.088222	1.807113
H	-4.162608	0.441181	-1.199334
H	-5.288145	0.759616	0.095626
C	-1.073665	-0.658527	2.507510
H	-1.551385	0.211325	2.956831
H	-0.002921	-0.761341	2.678056
C	-1.842048	-1.854942	2.388980
H	-2.879650	-1.810150	2.708606
H	-1.350007	-2.796170	2.614569
H	-0.470705	1.766942	-2.310344
H	0.215473	1.919352	2.256417
C	-2.118822	2.892879	-1.554671
H	-2.361167	3.345291	-2.520851
H	-2.768071	2.022399	-1.424435
H	-2.380371	3.622477	-0.782939
C	0.258021	3.715664	-1.794970
H	1.324403	3.467538	-1.782357

H	0.036508	4.122126	-2.786758
H	0.086865	4.519573	-1.072252
C	1.509158	3.358456	1.357952
H	1.538711	4.115355	0.570167
H	1.680994	3.877154	2.306271
H	2.350472	2.674146	1.216511
C	-0.987113	3.593062	1.677254
H	-1.955980	3.084288	1.722667
H	-0.842390	4.105284	2.632754
H	-1.043739	4.363997	0.902088
O	0.475702	-3.266850	-1.179347
C	0.732265	-4.654239	-1.315253
H	0.387003	-5.221636	-0.442702
H	0.178750	-4.985823	-2.194432
H	1.799411	-4.866065	-1.482945
O	0.948583	-3.283690	1.091401
C	1.953671	-4.167661	1.571076
H	2.719783	-3.633308	2.146965
H	1.453238	-4.872145	2.237369
H	2.442302	-4.739288	0.773395
O	2.702359	-0.937743	-0.731011

L28 – Hexene

Electronic Energy: -1871.42382730
Enthalpy: -1870.957851
Free Energy: -1871.048391

Cr	-1.372431	-0.712188	-0.492447
P	-0.222492	1.300295	0.205568
N	1.444920	0.686663	0.203335
C	1.651454	-0.581021	-0.195486
N	0.647622	-1.421299	-0.345937
H	2.248676	1.301075	0.269300
C	1.176138	-2.669656	-0.907777
C	2.993375	-1.133818	-0.550368
C	2.610671	-2.353813	-1.380574
H	3.283628	-3.203378	-1.261594
H	2.590520	-2.097989	-2.442303
H	-2.743004	-1.611677	-0.535561
H	-1.975601	0.326271	-2.817528
H	-2.727397	1.414378	-1.553975
C	-3.340148	-0.668284	-1.424214
C	-2.463050	0.397390	-1.843395
C	-4.508075	-0.324319	-0.507133
H	-4.301984	0.652120	-0.043905
H	-5.408696	-0.188130	-1.117453
C	-4.762263	-1.342143	0.601648
H	-5.025809	-2.315707	0.164955
H	-5.630395	-1.026214	1.188317
C	-3.547241	-1.507229	1.513235
H	-3.261234	-0.513912	1.899066
H	-3.813009	-2.101804	2.396853
C	-2.361710	-2.146493	0.802212
H	-1.457167	-2.159254	1.423226
H	-2.563808	-3.183804	0.516443
H	-3.554171	-1.442142	-2.168237
C	-0.426011	3.859749	0.683941
C	-0.230001	3.163616	2.013481
H	0.183252	4.765080	0.596727
H	-1.479859	4.140304	0.534667
H	0.823998	3.205974	2.335898
H	-0.845546	3.597287	2.806529
N	-0.647179	1.780452	1.762156
N	-0.002532	2.880711	-0.321344
C	-0.517388	0.841478	2.862690
H	-0.819671	-0.160496	2.538889

H	0.513911	0.779529	3.240022
H	-1.171797	1.139382	3.686186
C	-0.136616	3.254688	-1.717666
H	-1.164680	3.537237	-1.981368
H	0.517927	4.104064	-1.935274
H	0.169198	2.425837	-2.361120
H	3.607042	-0.407453	-1.088464
H	3.532966	-1.403865	0.363349
C	0.299506	-3.105809	-2.089447
F	0.902892	-4.040577	-2.826080
F	0.050150	-2.043122	-2.890153
F	-0.895067	-3.585672	-1.697099
C	1.211278	-3.757070	0.176180
F	1.587450	-4.934917	-0.342705
F	0.033327	-3.930265	0.784922
F	2.106506	-3.411102	1.123335

L28 – Octene

Electronic Energy: -1950.03043660
Enthalpy: -1949.501395
Free Energy: -1949.595108

24	-1.375610	-0.628000	0.405323
15	-0.012047	1.375474	0.057802
7	1.579685	0.704105	-0.233475
6	1.765775	-0.633348	-0.251297
7	0.785964	-1.493101	-0.105579
1	2.385111	1.285678	-0.435859
6	1.375525	-2.836447	-0.152601
6	3.134571	-1.216644	-0.408048
6	2.827108	-2.682065	-0.658969
1	3.507459	-3.373851	-0.161369
1	2.862474	-2.904216	-1.727004
6	-2.697336	-2.358369	0.571836
6	-2.761902	-2.022961	-0.921771
6	-4.156269	-1.691058	-1.437596
6	-4.828113	-0.517835	-0.739738
6	-2.964283	0.748447	0.468190
6	-3.963901	0.738117	-0.679160
1	-3.706929	-2.457114	0.963992
1	-2.097408	-1.182160	-1.284167
1	-4.775443	-2.590354	-1.343942
1	-5.767715	-0.306322	-1.260679
1	-2.537076	1.754399	0.589275
1	-2.143453	-3.277970	0.737586
1	-2.326733	-2.860925	-1.473143
1	-4.082624	-1.481219	-2.512111
1	-5.115070	-0.799752	0.283788
1	-3.492361	0.543186	1.410185
1	-3.458293	0.873384	-1.649010
1	-4.623492	1.612463	-0.579568
6	-1.153585	-0.554359	2.456253
1	-1.420023	0.454382	2.768058
1	-0.159377	-0.902134	2.738064
6	-2.195559	-1.519543	2.389712
1	-3.201934	-1.177233	2.609554
1	-1.990911	-2.527717	2.732264
1	3.698608	-1.051865	0.516450
1	3.695793	-0.738620	-1.215180
6	0.377498	3.877672	0.665343
6	-0.381984	3.869916	-0.641620
1	1.455837	4.042178	0.498050
1	0.021709	4.652556	1.350610
1	0.018512	4.598756	-1.354152
1	-1.448948	4.095495	-0.487230
7	-0.205592	2.516173	-1.166013

7	0.139245	2.554312	1.252227
6	-0.872847	2.198600	-2.413409
1	-0.443210	2.793562	-3.225452
1	-0.723028	1.144568	-2.666074
1	-1.952393	2.400890	-2.374502
6	0.869863	2.277498	2.476813
1	1.948492	2.464087	2.362538
1	0.497316	2.914746	3.283914
1	0.737130	1.237529	2.779527
6	0.605950	-3.750578	-1.115828
6	1.371194	-3.418960	1.264715
9	1.801432	-4.687013	1.278599
9	2.187755	-2.691075	2.052907
9	0.150648	-3.387609	1.826785
9	1.337932	-4.827297	-1.433275
9	-0.556717	-4.197630	-0.606604
9	0.323718	-3.091910	-2.253551

L29 – Hexene

Electronic Energy: -1276.04653981
Enthalpy: -1275.538558
Free Energy: -1275.621744

Cr	-1.352849	-0.614718	-0.491953
P	-0.141480	1.370051	0.200905
N	1.491074	0.722528	0.224463
C	1.643185	-0.562208	-0.186057
N	0.614565	-1.341645	-0.385303
H	2.316609	1.305118	0.299521
C	1.086920	-2.663146	-0.905122
C	2.966494	-1.192109	-0.486543
C	2.534994	-2.370908	-1.353793
H	3.183057	-3.244166	-1.253058
H	2.541087	-2.074619	-2.408267
H	-2.685761	-1.563989	-0.607598
H	-2.150910	0.791626	-2.578576
H	-2.867108	1.574897	-1.090056
C	-3.364329	-0.530569	-1.329289
C	-2.571299	0.647000	-1.582170
C	-4.525092	-0.433621	-0.346209
H	-4.361598	0.449705	0.288468
H	-5.447291	-0.239469	-0.906633
C	-4.692258	-1.655786	0.552587
H	-4.898205	-2.545911	-0.058989
H	-5.569553	-1.516979	1.191871
C	-3.455403	-1.903998	1.413609
H	-3.238540	-0.985703	1.983303
H	-3.665185	-2.674506	2.166515
C	-2.228857	-2.302353	0.597170
H	-1.326238	-2.343791	1.218808
H	-2.352581	-3.294203	0.145308
H	-3.555635	-1.175585	-2.193057
C	-0.365384	3.948398	0.560261
C	-0.198921	3.317935	1.925859
H	0.228842	4.861291	0.448401
H	-1.420252	4.201468	0.368759
H	0.845435	3.386578	2.273814
H	-0.839893	3.782698	2.680566
N	-0.600018	1.923109	1.725360
N	0.110051	2.933025	-0.381509
C	-0.518691	1.035834	2.869760
H	-0.821797	0.023780	2.580934
H	0.497603	0.977945	3.286802
H	-1.197137	1.377841	3.656191
C	0.005347	3.241467	-1.795737
H	-1.023292	3.474730	-2.104478

H	0.636049	4.104310	-2.030378
H	0.363244	2.398690	-2.392890
C	0.190069	-3.079360	-2.057898
H	0.566720	-3.987987	-2.537478
H	-0.827729	-3.292745	-1.712305
H	0.142081	-2.294965	-2.822519
C	1.055232	-3.700031	0.211749
H	0.040225	-3.861134	0.582962
H	1.428355	-4.661369	-0.153928
H	1.681163	-3.397930	1.057669
H	3.657290	-0.499495	-0.974809
H	3.444747	-1.507579	0.449138

L29 – Octene

Electronic Energy: -1354.65131078
Enthalpy: -1354.080910
Free Energy: -1354.165412

Cr	-1.317702	-0.569649	0.365530
P	0.038421	1.432506	0.051542
N	1.608253	0.724463	-0.186647
C	1.732444	-0.633171	-0.221481
N	0.717661	-1.444368	-0.140894
H	2.437593	1.274430	-0.378124
C	1.232409	-2.850890	-0.150260
C	3.078594	-1.283845	-0.294749
C	2.702760	-2.721767	-0.611750
H	3.348261	-3.458093	-0.127265
H	2.763969	-2.894518	-1.691003
C	-2.494438	-2.399341	0.459447
C	-2.644115	-1.974375	-1.005297
C	-4.078544	-1.697597	-1.436457
C	-4.783931	-0.614776	-0.632949
C	-2.951211	0.746357	0.519654
C	-4.018277	0.704161	-0.565479
H	-3.473428	-2.645479	0.865817
H	-2.040526	-1.077856	-1.338473
H	-4.638138	-2.637986	-1.372710
H	-5.773494	-0.457377	-1.074672
H	-2.554644	1.767928	0.616664
H	-1.838019	-3.264020	0.552675
H	-2.186546	-2.750143	-1.628889
H	-4.071757	-1.416707	-2.497142
H	-4.970564	-0.968769	0.391867
H	-3.418479	0.525068	1.490942
H	-3.584427	0.918142	-1.555968
H	-4.738922	1.516552	-0.391970
C	-1.063794	-0.584627	2.414331
H	-1.382994	0.392148	2.773875
H	-0.047784	-0.884819	2.670625
C	-2.052437	-1.601607	2.306058
H	-3.075978	-1.326824	2.542896
H	-1.791720	-2.611871	2.608740
H	3.575525	-1.171817	0.677390
H	3.732253	-0.812362	-1.034589
C	0.417599	3.948687	0.603717
C	-0.331966	3.909638	-0.708863
H	1.497959	4.105080	0.440872
H	0.058714	4.742805	1.265185
H	0.066121	4.629031	-1.432395
H	-1.401509	4.129526	-0.562024
N	-0.140963	2.547578	-1.204965
N	0.163946	2.642434	1.219620
C	-0.844382	2.187148	-2.420694
H	-0.473135	2.788455	-3.256258
H	-0.658125	1.136831	-2.666383

H	-1.930594	2.343046	-2.342760
C	0.854248	2.393405	2.471606
H	1.944132	2.516535	2.378125
H	0.496907	3.090799	3.234724
H	0.655944	1.379441	2.823375
C	0.448739	-3.708524	-1.130407
H	0.950634	-4.672274	-1.261901
H	-0.565918	-3.922601	-0.785908
H	0.390111	-3.226950	-2.111614
C	1.134407	-3.406383	1.265214
H	0.104873	-3.354305	1.636273
H	1.447145	-4.454568	1.294951
H	1.770040	-2.846139	1.959479

L30 – Hexene

Electronic Energy: -1354.66847169
Enthalpy: -1354.101512
Free Energy: -1354.189402

Cr	-1.349643	-0.654310	-0.548924
P	-0.157104	1.333127	0.134414
N	1.468147	0.685040	0.236711
C	1.641182	-0.599684	-0.171999
N	0.623478	-1.379684	-0.413495
H	2.289426	1.270735	0.341478
C	1.108001	-2.692946	-0.939048
C	3.006554	-1.210958	-0.388613
C	2.607682	-2.446490	-1.215460
H	3.219801	-3.320017	-0.974160
H	2.755557	-2.232282	-2.280178
H	-2.728272	-1.545033	-0.553712
H	-2.229586	0.711983	-2.626129
H	-2.799002	1.589599	-1.127598
C	-3.412241	-0.495056	-1.238395
C	-2.583234	0.628778	-1.596952
C	-4.468248	-0.307881	-0.156117
H	-4.176956	0.553631	0.464076
H	-5.417311	-0.033514	-0.632027
C	-4.653688	-1.523226	0.747946
H	-4.959004	-2.391798	0.146835
H	-5.473994	-1.334503	1.447182
C	-3.379919	-1.857862	1.520650
H	-3.080060	-0.966823	2.095740
H	-3.583322	-2.635690	2.267821
C	-2.226411	-2.299252	0.622886
H	-1.290240	-2.381492	1.187009
H	-2.421108	-3.284017	0.180045
H	-3.717899	-1.151641	-2.059316
C	-0.408484	3.912968	0.468962
C	-0.303067	3.290861	1.844763
H	0.187247	4.827314	0.379691
H	-1.454073	4.161847	0.227758
H	0.723222	3.367719	2.241289
H	-0.981321	3.756648	2.565489
N	-0.686712	1.892814	1.634082
N	0.113105	2.894372	-0.444712
C	-0.653282	1.011172	2.785578
H	-0.936406	-0.004339	2.487361
H	0.342392	0.961584	3.250768
H	-1.370841	1.351737	3.537403
C	0.066888	3.193053	-1.864210
H	-0.950068	3.411162	-2.219579
H	0.695967	4.062765	-2.076283
H	0.461902	2.351456	-2.439709
C	3.946653	-0.277129	-1.144978
C	3.624833	-1.572024	0.967469

H	4.874180	-0.801403	-1.391082
H	3.506386	0.077637	-2.082129
H	4.227280	0.596466	-0.545828
H	3.805237	-0.677957	1.573274
H	2.987955	-2.245175	1.547709
H	4.587634	-2.068344	0.815373
C	0.329852	-3.002515	-2.209293
H	0.677488	-3.933218	-2.667884
H	-0.739507	-3.126512	-1.993835
H	0.443280	-2.201042	-2.948003
C	0.888512	-3.798153	0.088444
H	-0.174270	-3.985982	0.257008
H	1.332856	-4.731860	-0.269116
H	1.347006	-3.557887	1.052079

L30 – Octene
Electronic Energy: -1433.27444330
Enthalpy: -1432.645086
Free Energy: -1432.734748

Cr	-1.335189	-0.581654	0.333899
P	0.022006	1.414987	-0.017078
N	1.548727	0.699352	-0.429744
C	1.695984	-0.656727	-0.372281
N	0.697307	-1.465847	-0.174486
H	2.366998	1.251673	-0.660948
C	1.216233	-2.866596	-0.107761
C	3.075028	-1.277578	-0.438068
C	2.695908	-2.760642	-0.542494
H	3.346039	-3.399570	0.062437
H	2.797722	-3.092697	-1.581529
C	-2.533164	-2.399899	0.467505
C	-2.676486	-2.005796	-1.006128
C	-4.107197	-1.723170	-1.445724
C	-4.803818	-0.618398	-0.664650
C	-2.962235	0.746457	0.470112
C	-4.024961	0.693765	-0.619244
H	-3.516030	-2.620672	0.879274
H	-2.061762	-1.124662	-1.357765
H	-4.676148	-2.656579	-1.364812
H	-5.790147	-0.458976	-1.112854
H	-2.562794	1.768064	0.554373
H	-1.892347	-3.274206	0.578111
H	-2.226615	-2.799673	-1.612273
H	-4.095698	-1.463033	-2.511644
H	-4.997895	-0.951440	0.365703
H	-3.434623	0.541689	1.442411
H	-3.583842	0.883072	-1.611350
H	-4.738006	1.516985	-0.466009
C	-1.069969	-0.570378	2.381042
H	-1.363082	0.420239	2.725576
H	-0.057752	-0.888102	2.632114
C	-2.077796	-1.570532	2.296546
H	-3.095552	-1.271828	2.529673
H	-1.835957	-2.578710	2.620818
C	0.487060	3.889972	0.654680
C	-0.356712	3.938175	-0.599198
H	1.554951	4.042824	0.420820
H	0.191499	4.647847	1.386078
H	0.000514	4.693798	-1.306985
H	-1.409117	4.162855	-0.363567
N	-0.222821	2.606744	-1.187592
N	0.259951	2.551995	1.209512
C	-0.998652	2.335817	-2.382046
H	-0.658476	2.980862	-3.198179
H	-0.849206	1.299861	-2.700833

H	-2.074986	2.507442	-2.234995
C	1.059617	2.214906	2.373017
H	2.136743	2.352905	2.190159
H	0.773527	2.849629	3.216781
H	0.896628	1.175269	2.664750
C	0.448692	-3.759206	-1.072458
H	0.928938	-4.740771	-1.134223
H	-0.583688	-3.926921	-0.754774
H	0.436815	-3.329626	-2.079272
C	1.071432	-3.378584	1.320834
H	0.026508	-3.347670	1.646597
H	1.410272	-4.416618	1.393377
H	1.661497	-2.785138	2.026398
C	3.814833	-0.942940	0.863919
H	4.779332	-1.458239	0.888819
H	4.012048	0.131197	0.947821
H	3.249049	-1.248219	1.750163
C	3.894905	-0.795540	-1.631818
H	4.161305	0.264701	-1.554770
H	4.835564	-1.351528	-1.683590
H	3.368157	-0.946347	-2.578757

L31 – Hexene

Electronic Energy: -1395.88486533
Enthalpy: -1395.449392
Free Energy: -1395.528903

Cr	-1.390835	-0.528968	-0.470417
P	-0.134899	1.444600	0.195102
N	1.522919	0.809136	0.051491
C	1.657088	-0.486974	-0.266828
N	0.597570	-1.257280	-0.393908
H	2.352096	1.390270	0.099513
C	1.035636	-2.573771	-0.764506
C	2.959446	-1.182543	-0.517868
C	2.496139	-2.480411	-1.175978
H	3.050828	-3.365128	-0.865764
H	2.544624	-2.405396	-2.263720
H	-2.663595	-1.511465	-0.784668
H	-2.240149	1.087225	-2.396118
H	-2.988499	1.645961	-0.826026
C	-3.389563	-0.433961	-1.332435
C	-2.648685	0.800069	-1.426630
C	-4.549545	-0.525677	-0.348636
H	-4.424839	0.265035	0.405789
H	-5.479971	-0.294785	-0.880712
C	-4.658610	-1.871040	0.363322
H	-4.829328	-2.670624	-0.371432
H	-5.536797	-1.864214	1.016140
C	-3.406262	-2.189304	1.177131
H	-3.224488	-1.357971	1.878640
H	-3.579419	-3.070472	1.808450
C	-2.169967	-2.413627	0.315278
H	-1.265097	-2.538614	0.919153
H	-2.260540	-3.310454	-0.307547
H	-3.554145	-0.965172	-2.275183
H	3.635117	-0.583859	-1.133398
H	3.468496	-1.355853	0.436772
C	-0.293593	4.019250	0.588782
C	0.001587	3.378027	1.928147
H	0.298978	4.924593	0.421301
H	-1.358738	4.286169	0.504595
H	1.074203	3.439358	2.175852
H	-0.563362	3.837973	2.743848
N	-0.423896	1.986406	1.756969
N	0.071571	3.004212	-0.402696

C	-0.278641	1.086187	2.885056
H	-0.633118	0.086284	2.612092
H	0.764826	0.997232	3.220424
H	-0.883281	1.439845	3.724319
C	-0.158596	3.325145	-1.799431
H	-1.211019	3.555846	-2.014573
H	0.445675	4.193629	-2.078065
H	0.152253	2.490411	-2.433083
F	0.226982	-3.048583	-1.754625
F	0.863179	-3.426440	0.292042

L31 – Octene

Electronic Energy: -1474.497673
Enthalpy: -1473.999863
Free Energy: -1474.082525

24	-1.271832	-0.564892	0.496854
15	0.029486	1.458480	0.055200
7	1.590092	0.749619	-0.398719
6	1.701552	-0.589835	-0.457942
7	0.682449	-1.371327	-0.194634
1	2.420843	1.307720	-0.559855
6	1.104941	-2.729149	-0.333231
6	2.966444	-1.302952	-0.828182
6	2.615561	-2.757863	-0.529000
1	3.079690	-3.099293	0.397384
1	2.889330	-3.451534	-1.322981
6	-2.311900	-2.452241	0.232135
6	-2.539292	-1.750028	-1.113403
6	-3.990988	-1.429116	-1.437547
6	-4.686444	-0.527917	-0.427051
6	-2.884437	0.683625	0.918586
6	-3.959145	0.789176	-0.153251
1	-3.257333	-2.865554	0.577878
1	-1.958393	-0.798841	-1.291433
1	-4.535880	-2.375683	-1.531866
1	-5.700156	-0.332033	-0.791917
1	-2.496015	1.684023	1.161989
1	-1.575918	-3.247275	0.128011
1	-2.086056	-2.384100	-1.882848
1	-4.024632	-0.956948	-2.427899
1	-4.812476	-1.065703	0.525098
1	-3.332277	0.300365	1.848339
1	-3.535902	1.178284	-1.094510
1	-4.701925	1.540777	0.151280
6	-0.957431	-0.978214	2.476259
1	-1.305265	-0.119882	3.047684
1	0.075786	-1.280305	2.644290
6	-1.907346	-2.001024	2.171200
1	-2.935235	-1.824641	2.476109
1	-1.592201	-3.035054	2.272525
1	3.821882	-0.926140	-0.261634
1	3.186129	-1.125990	-1.886503
6	0.071137	4.016401	0.572097
6	0.064877	3.857368	-0.934296
1	0.780526	4.779990	0.906959
1	-0.928787	4.289594	0.942910
1	1.080792	3.953311	-1.353391
1	-0.575929	4.594095	-1.426889
7	-0.476454	2.512796	-1.146864
7	0.479249	2.706656	1.088605
6	-0.646239	2.048019	-2.508794
1	0.298114	2.034525	-3.072866
1	-1.053135	1.030050	-2.502714
1	-1.355980	2.691682	-3.035846
6	0.476310	2.521442	2.528883

1	1.177501	3.223416	2.989064
1	-0.515613	2.682359	2.974851
1	0.807603	1.508852	2.774215
9	0.433237	-3.302206	-1.385329
9	0.709032	-3.441295	0.766408

L32 – Hexene
Electronic Energy: -1594.32313933
Enthalpy: -1593.902538
Free Energy: -1593.985983

Cr	-1.403441	-0.528027	-0.452082
P	-0.142608	1.459032	0.206548
N	1.527504	0.802400	0.067477
C	1.628137	-0.486370	-0.249859
N	0.586480	-1.270083	-0.390394
H	2.375191	1.361106	0.096747
C	1.035192	-2.580942	-0.791131
C	2.942058	-1.211371	-0.500617
C	2.496716	-2.474019	-1.202333
H	3.079406	-3.347131	-0.913260
H	2.559584	-2.328437	-2.281424
H	-2.667461	-1.515967	-0.774563
H	-2.249619	1.095434	-2.370847
H	-3.011045	1.638313	-0.800978
C	-3.397821	-0.439414	-1.326336
C	-2.664300	0.799038	-1.406817
C	-4.565863	-0.547892	-0.354254
H	-4.458176	0.240504	0.404985
H	-5.492246	-0.324091	-0.896122
C	-4.669117	-1.898157	0.349125
H	-4.822236	-2.695808	-0.391437
H	-5.554816	-1.904179	0.991421
C	-3.423216	-2.205578	1.176400
H	-3.257968	-1.375553	1.883284
H	-3.592679	-3.091351	1.801979
C	-2.174817	-2.414097	0.328910
H	-1.275157	-2.522633	0.944810
H	-2.243618	-3.312889	-0.293854
H	-3.547009	-0.968369	-2.272913
C	-0.256644	4.036305	0.583404
C	0.032997	3.396606	1.924882
H	0.358685	4.923866	0.404738
H	-1.314725	4.329613	0.503972
H	1.106450	3.440970	2.169937
H	-0.523310	3.867958	2.739748
N	-0.413722	2.009125	1.763494
N	0.071714	3.005341	-0.406371
C	-0.289158	1.114915	2.899960
H	-0.658861	0.118904	2.633239
H	0.750701	1.012084	3.240469
H	-0.892955	1.486241	3.731920
C	-0.151289	3.323409	-1.805114
H	-1.198429	3.576923	-2.019087
H	0.472981	4.175809	-2.088293
H	0.140331	2.478650	-2.434245
F	0.235013	-3.022333	-1.798200
F	0.866019	-3.453479	0.239408
F	3.793671	-0.439640	-1.219292
F	3.541830	-1.461284	0.695433

L32 – Octene
Electronic Energy: -1672.93517026
Enthalpy: -1672.452703
Free Energy: -1672.540501

Cr	-1.294836	-0.615745	0.527448
P	0.017283	1.421859	0.082973
N	1.570003	0.682401	-0.416745
C	1.650347	-0.649537	-0.447834
N	0.662752	-1.448765	-0.142846
H	2.415344	1.211866	-0.607542
C	1.111709	-2.808845	-0.255906
C	2.907266	-1.395159	-0.874788
C	2.623249	-2.814264	-0.439439
H	3.104536	-3.006276	0.520461
H	2.953785	-3.552293	-1.168248
C	-2.317795	-2.506632	0.226545
C	-2.510362	-1.801231	-1.125014
C	-3.950354	-1.465199	-1.485282
C	-4.672427	-0.566469	-0.491120
C	-2.912213	0.620872	0.923246
C	-3.950150	0.744845	-0.181310
H	-3.270400	-2.929453	0.539482
H	-1.907415	-0.862908	-1.298407
H	-4.499094	-2.406958	-1.602131
H	-5.671900	-0.362598	-0.889161
H	-2.526457	1.614423	1.198179
H	-1.577237	-3.299310	0.138870
H	-2.050151	-2.446828	-1.880803
H	-3.952563	-0.987118	-2.473275
H	-4.835869	-1.110799	0.451276
H	-3.388365	0.221336	1.831260
H	-3.495767	1.144022	-1.103520
H	-4.698829	1.495752	0.109475
C	-1.026826	-1.050100	2.506256
H	-1.386169	-0.197879	3.080121
H	0.001100	-1.356433	2.698358
C	-1.971450	-2.069710	2.170139
H	-3.005993	-1.894250	2.452800
H	-1.659611	-3.104061	2.278288
C	0.122017	3.974151	0.604502
C	0.082045	3.819273	-0.901283
H	0.856908	4.718862	0.925874
H	-0.862492	4.268385	0.998379
H	1.090004	3.896870	-1.340795
H	-0.556337	4.567031	-1.379745
N	-0.485855	2.483036	-1.108174
N	0.509299	2.652539	1.110327
C	-0.688740	2.029208	-2.470275
H	0.244180	2.005136	-3.051290
H	-1.111410	1.018523	-2.463675
H	-1.399657	2.686705	-2.977807
C	0.554804	2.469339	2.550440
H	1.275209	3.168928	2.983194
H	-0.420060	2.636965	3.029305
H	0.892369	1.457662	2.789178
F	4.016320	-0.846669	-0.319261
F	3.039251	-1.276982	-2.226194
F	0.722981	-3.496016	0.854101
F	0.467646	-3.405935	-1.303019

L33 – Hexene (PNCN_S_PCpNMe_X-H_Z-CF3-TS1)
Electronic Energy: -1871.41447720
Enthalpy: -1870.947915
Free Energy: -1871.040413

Cr	-1.407209	-0.479269	-0.527051
P	-0.138943	1.482015	0.138912
N	1.497550	0.832407	-0.046528
C	1.600085	-0.486264	-0.307510

N	0.558058	-1.252414	-0.470897
H	2.342332	1.380407	0.068638
C	0.985191	-2.636309	-0.704511
C	2.924041	-1.226095	-0.379086
C	2.486321	-2.566432	-0.992081
H	3.048409	-3.407899	-0.584118
H	2.668888	-2.540348	-2.068614
H	-2.669695	-1.477069	-0.826945
H	-2.285942	1.158134	-2.422022
H	-3.023732	1.686341	-0.836029
C	-3.413875	-0.387243	-1.369992
C	-2.686393	0.853076	-1.454851
C	-4.566680	-0.505584	-0.380694
H	-4.445910	0.274809	0.384784
H	-5.502067	-0.275556	-0.904299
C	-4.661524	-1.862434	0.311594
H	-4.827631	-2.653122	-0.433869
H	-5.537792	-1.873183	0.966696
C	-3.405769	-2.181341	1.119813
H	-3.227438	-1.356822	1.829531
H	-3.570348	-3.071226	1.740692
C	-2.168331	-2.381800	0.250941
H	-1.262941	-2.493559	0.860468
H	-2.251003	-3.281707	-0.370072
H	-3.576434	-0.912316	-2.316640
C	-0.229570	4.038037	0.648938
C	0.123352	3.330215	1.939632
H	0.382043	4.931077	0.484524
H	-1.288249	4.340007	0.639884
H	1.210527	3.348803	2.123456
H	-0.375559	3.771497	2.806815
N	-0.356923	1.958891	1.738863
N	0.041025	3.058296	-0.407494
C	-0.108545	0.999464	2.800122
H	-0.556971	0.034456	2.539363
H	0.964824	0.838492	2.985613
H	-0.573247	1.344259	3.727180
C	-0.268778	3.446782	-1.771481
H	-1.328438	3.702843	-1.907622
H	0.332754	4.317829	-2.047389
H	-0.012616	2.638649	-2.460620
C	3.941871	-0.507984	-1.265502
F	4.993353	-1.283796	-1.533264
F	4.394216	0.627617	-0.694379
F	3.363820	-0.169180	-2.432064
C	3.459969	-1.414060	1.047521
F	3.611043	-0.242072	1.689455
F	4.635248	-2.046659	1.049761
F	2.584924	-2.149333	1.760807
H	0.419571	-3.064993	-1.536051
H	0.761552	-3.237075	0.184147

L33 – Octene (PNCN_S_PCpNMe_X-H_Z-CF3-TS2)
Electronic Energy: -1950.02348191
Enthalpy: -1949.495097
Free Energy: -1949.589773

24	-1.348433	-0.552477	0.270156
15	0.016987	1.457142	-0.040551
7	1.545643	0.705171	-0.499925
6	1.648347	-0.643639	-0.426760
7	0.631908	-1.427607	-0.230909
1	2.384431	1.238228	-0.701906
6	1.091308	-2.809111	-0.088599
6	2.992991	-1.359957	-0.441771
6	2.553025	-2.827836	-0.542529

1	3.184886	-3.490771	0.050027
1	2.624429	-3.150258	-1.583068
1	0.467833	-3.476209	-0.691651
6	-2.304764	-2.494332	0.245248
6	-2.556002	-1.981117	-1.177976
6	-4.027359	-1.805781	-1.528002
6	-4.773013	-0.828571	-0.629454
6	-3.028452	0.660186	0.505996
6	-4.126150	0.553611	-0.543811
1	-3.227466	-2.912161	0.642647
1	-2.052457	-1.011096	-1.464082
1	-4.505672	-2.791403	-1.491660
1	-5.799210	-0.744603	-1.001745
1	-2.682113	1.701787	0.588665
1	-1.530015	-3.260861	0.256560
1	-2.055930	-2.665083	-1.872878
1	-4.098175	-1.468180	-2.569369
1	-4.859985	-1.245072	0.385395
1	-3.444899	0.410571	1.493557
1	-3.745093	0.833417	-1.539664
1	-4.909427	1.293077	-0.323332
6	-1.033831	-0.694414	2.302752
1	-1.397078	0.239704	2.728324
1	0.000820	-0.953557	2.528133
6	-1.963266	-1.759692	2.134726
1	-3.003193	-1.556241	2.374996
1	-1.647002	-2.767678	2.387165
1	0.980972	-3.117834	0.958979
6	0.609870	3.889768	0.649126
6	-0.265629	3.997004	-0.579239
1	1.677208	3.991506	0.388902
1	0.371642	4.649404	1.398718
1	0.111853	4.737888	-1.291550
1	-1.296963	4.273759	-0.310871
7	-0.227980	2.664281	-1.184542
7	0.330588	2.555581	1.193465
6	-1.067859	2.443673	-2.346862
1	-0.741153	3.091525	-3.165620
1	-0.971475	1.410007	-2.691495
1	-2.128671	2.651686	-2.145201
6	1.119308	2.162151	2.348802
1	2.199170	2.259776	2.164219
1	0.858932	2.790120	3.205276
1	0.913812	1.123174	2.617409
6	3.695812	-1.088044	0.896603
6	3.868433	-0.956156	-1.626557
9	4.831316	-1.779927	1.010773
9	3.980943	0.213461	1.070453
9	2.877686	-1.456941	1.905837
9	4.252860	0.335576	-1.554828
9	4.967322	-1.710180	-1.700945
9	3.181246	-1.104899	-2.772052

L34 – Hexene

Electronic Energy: -1276.04167904
Enthalpy: -1275.533062
Free Energy: -1275.616961

Cr	-1.390302	-0.482557	-0.612307
P	-0.124686	1.474660	0.046760
N	1.503063	0.832229	-0.082631
C	1.621114	-0.487887	-0.364854
N	0.567190	-1.237189	-0.557943
H	2.343246	1.390565	0.015963
C	1.012457	-2.622646	-0.787633
C	2.944135	-1.219929	-0.393771

C	2.503091	-2.514342	-1.100320
H	3.075176	-3.384951	-0.770427
H	2.652256	-2.409512	-2.180519
H	-2.698095	-1.453574	-0.784613
H	-2.431585	1.153065	-2.438465
H	-2.998129	1.710134	-0.792670
C	-3.467139	-0.365050	-1.259383
C	-2.735595	0.865052	-1.431548
C	-4.504978	-0.462701	-0.148831
H	-4.248102	0.269639	0.631574
H	-5.478757	-0.153209	-0.546860
C	-4.599390	-1.848887	0.482501
H	-4.855415	-2.589696	-0.288676
H	-5.421961	-1.865307	1.204143
C	-3.299315	-2.254863	1.173231
H	-3.065404	-1.498193	1.938608
H	-3.443596	-3.194043	1.722919
C	-2.115651	-2.393206	0.218383
H	-1.178103	-2.520268	0.771347
H	-2.223314	-3.271038	-0.430719
H	-3.742686	-0.891421	-2.178766
C	-0.304143	4.028624	0.553997
C	-0.024318	3.329346	1.867183
H	0.283760	4.944941	0.437207
H	-1.370090	4.292480	0.467219
H	1.047582	3.374968	2.123713
H	-0.592033	3.758480	2.697821
N	-0.458311	1.950519	1.630506
N	0.084967	3.062299	-0.475127
C	-0.292055	0.996010	2.709610
H	-0.679120	0.017607	2.401722
H	0.760173	0.866837	3.006817
H	-0.860631	1.320041	3.585415
C	-0.119261	3.444932	-1.859901
H	-1.167595	3.686957	-2.084431
H	0.490734	4.323719	-2.089832
H	0.201697	2.637854	-2.523723
C	4.041810	-0.468837	-1.134559
C	3.363727	-1.481742	1.059536
H	0.430303	-3.074229	-1.595831
H	0.817889	-3.218547	0.114368
H	4.937721	-1.092064	-1.205682
H	3.742441	-0.201193	-2.152154
H	4.337396	0.448305	-0.613076
H	3.533699	-0.545967	1.602300
H	2.605940	-2.052178	1.606461
H	4.295605	-2.053684	1.081828

L34 – Octene

Electronic Energy: -1354.64960528
Enthalpy: -1354.078759
Free Energy: -1354.164960

Cr	-1.273104	-0.561173	0.484813
P	0.033458	1.453515	0.047349
N	1.571035	0.720624	-0.351110
C	1.660225	-0.635383	-0.411665
N	0.625645	-1.405402	-0.227678
H	2.412650	1.262812	-0.511143
C	1.076335	-2.803339	-0.279671
C	2.982654	-1.352713	-0.593315
C	2.463282	-2.762897	-0.918836
H	3.129224	-3.548308	-0.553068
H	2.376373	-2.881575	-2.004351
H	0.366146	-3.408983	-0.851759

C	-2.298004	-2.463800	0.265983
C	-2.539262	-1.787442	-1.092407
C	-3.998551	-1.500167	-1.416151
C	-4.703654	-0.588030	-0.421510
C	-2.912679	0.656203	0.907327
C	-3.990780	0.740188	-0.164096
H	-3.238933	-2.876261	0.625583
H	-1.985553	-0.823638	-1.285665
H	-4.528624	-2.457219	-1.487331
H	-5.718058	-0.408750	-0.793209
H	-2.539007	1.663854	1.143328
H	-1.565995	-3.265010	0.169777
H	-2.078617	-2.421256	-1.858515
H	-4.044721	-1.049823	-2.415989
H	-4.829822	-1.112366	0.537756
H	-3.356151	0.275456	1.840405
H	-3.570745	1.122280	-1.110022
H	-4.742961	1.486603	0.129609
C	-0.922764	-0.946177	2.467124
H	-1.272220	-0.082251	3.029076
H	0.115960	-1.233034	2.633174
C	-1.869205	-1.980062	2.191702
H	-2.894408	-1.803920	2.505814
H	-1.553032	-3.012021	2.314882
H	1.094622	-3.212991	0.741231
C	0.041465	4.023290	0.517043
C	0.047307	3.840019	-0.986239
H	0.732332	4.808088	0.842424
H	-0.966153	4.282063	0.877949
H	1.066033	3.940209	-1.397400
H	-0.597171	4.562181	-1.495851
N	-0.477123	2.486620	-1.178304
N	0.480259	2.732451	1.051514
C	-0.613444	1.995445	-2.534087
H	0.345122	1.959377	-3.073643
H	-1.031017	0.982163	-2.520504
H	-1.302518	2.633486	-3.094470
C	0.504419	2.575684	2.493749
H	1.176923	3.319980	2.930133
H	-0.486873	2.696521	2.954370
H	0.892487	1.586923	2.754040
C	3.724387	-1.325900	0.749648
H	4.668316	-1.871638	0.664388
H	3.959519	-0.302555	1.060404
H	3.139059	-1.792993	1.548849
C	3.853296	-0.757115	-1.691176
H	4.217115	0.242935	-1.428845
H	4.736990	-1.381804	-1.849025
H	3.319023	-0.687839	-2.643749

L35 – Hexene (PNCN_S_PCpNMe_X-H_Z-F-TS1)
Electronic Energy: -1395.86178369
Enthalpy: -1395.425724
Free Energy: -1395.504855

Cr	-1.389139	-0.475472	-0.587693
P	-0.109315	1.479576	0.093292
N	1.512766	0.769408	0.134773
C	1.599564	-0.513739	-0.259915
N	0.572874	-1.242269	-0.595976
H	2.374535	1.290661	0.259386
C	1.035703	-2.596734	-0.957884
C	2.900612	-1.287910	-0.315986
C	2.543962	-2.473915	-1.175179
H	3.111492	-3.361817	-0.896953
H	2.767477	-2.223731	-2.215170

H	-2.716481	-1.417084	-0.746700
H	-2.529938	1.331256	-2.181614
H	-3.004728	1.710879	-0.458090
C	-3.499791	-0.307686	-1.117065
C	-2.780031	0.938355	-1.195754
C	-4.508577	-0.522364	0.003439
H	-4.234174	0.128410	0.847720
H	-5.491174	-0.178300	-0.339872
C	-4.582379	-1.966538	0.490620
H	-4.839334	-2.627306	-0.349687
H	-5.395783	-2.066517	1.215674
C	-3.269934	-2.422445	1.124329
H	-3.044756	-1.752684	1.967822
H	-3.393140	-3.419401	1.566431
C	-2.085206	-2.436226	0.159944
H	-1.143932	-2.567049	0.706118
H	-2.157137	-3.260885	-0.560228
H	-3.796333	-0.746861	-2.075061
C	-0.223697	4.064725	0.422983
C	-0.078217	3.439556	1.794672
H	0.415454	4.944471	0.296436
H	-1.266208	4.366811	0.236956
H	0.967539	3.466630	2.141695
H	-0.699179	3.936323	2.545464
N	-0.543523	2.063104	1.604409
N	0.189687	3.017865	-0.516850
C	-0.573527	1.180398	2.754195
H	-0.966129	0.200821	2.455692
H	0.419157	1.027361	3.201013
H	-1.240450	1.589130	3.518233
C	0.061763	3.310097	-1.933362
H	-0.966225	3.577085	-2.216514
H	0.717286	4.145133	-2.196919
H	0.373244	2.446406	-2.526661
F	3.926820	-0.526411	-0.775092
F	3.225044	-1.657179	0.962348
H	0.501776	-2.943448	-1.845403
H	0.796818	-3.288548	-0.141920

L35 – Octene (PNCN_S_PCpNMe_X-H_Z-F-TS2)
Electronic Energy: -1474.47048513
Enthalpy: -1473.973069
Free Energy: -1474.056857

Cr	-1.286245	-0.565038	0.500128
P	0.027657	1.459344	0.053187
N	1.558833	0.712663	-0.396766
C	1.634097	-0.635418	-0.417680
N	0.635846	-1.434897	-0.194286
H	2.411373	1.234448	-0.572230
C	1.117714	-2.826178	-0.218610
C	2.949167	-1.361950	-0.609431
C	2.520182	-2.790331	-0.831664
H	3.221903	-3.495949	-0.387012
H	2.478652	-2.971472	-1.908049
H	0.428634	-3.448345	-0.796924
C	-2.310627	-2.461880	0.236954
C	-2.524140	-1.770441	-1.118145
C	-3.974822	-1.467866	-1.465767
C	-4.691159	-0.560097	-0.475226
C	-2.918762	0.660414	0.898321
C	-3.973116	0.760446	-0.194131
H	-3.256279	-2.887247	0.567456
H	-1.957229	-0.810361	-1.291843
H	-4.510769	-2.419794	-1.557066
H	-5.697234	-0.369702	-0.863227

H	-2.536962	1.661465	1.149306
H	-1.570109	-3.256865	0.149353
H	-2.055185	-2.401150	-1.881863
H	-3.998218	-1.006852	-2.461444
H	-4.838239	-1.091924	0.476926
H	-3.382847	0.276345	1.819474
H	-3.532625	1.147627	-1.128358
H	-4.723950	1.510638	0.092770
C	-0.994483	-0.974538	2.486211
H	-1.349877	-0.109951	3.043559
H	0.035118	-1.273797	2.681440
C	-1.943063	-1.996698	2.176821
H	-2.975603	-1.814072	2.461902
H	-1.639387	-3.032163	2.302167
H	1.125385	-3.216721	0.806961
C	0.084737	4.021786	0.544377
C	0.065335	3.849023	-0.959851
H	0.800118	4.785861	0.865160
H	-0.910444	4.301514	0.922815
H	1.078838	3.933857	-1.385967
H	-0.574787	4.584671	-1.454967
N	-0.484203	2.504544	-1.156021
N	0.496159	2.715763	1.066489
C	-0.642762	2.027221	-2.515179
H	0.306691	2.002075	-3.069895
H	-1.055159	1.011869	-2.504826
H	-1.344704	2.668368	-3.055442
C	0.541377	2.549688	2.507657
H	1.243987	3.270497	2.935310
H	-0.438275	2.699145	2.983763
H	0.903351	1.548956	2.757270
F	3.684885	-1.203534	0.535658
F	3.686800	-0.822789	-1.616005

L36 – Hexene (PNCN_S_PCpNMe_X-OMe_TS1)
Electronic Energy: -1426.44647584
Enthalpy: -1425.926716
Free Energy: -1426.012781

Cr	-1.236125	-0.583173	-0.653404
P	-0.087060	1.404928	0.169207
N	1.594575	0.851732	0.046330
C	1.777487	-0.419964	-0.362518
N	0.751528	-1.219248	-0.509993
H	2.396733	1.466405	0.119358
C	1.192416	-2.511097	-1.030086
C	3.099321	-1.037976	-0.694290
C	2.678206	-2.315081	-1.419326
H	3.290637	-3.182702	-1.167959
H	2.726481	-2.173034	-2.501281
H	-2.534898	-1.567357	-0.851137
H	-2.131369	0.919248	-2.632607
H	-2.828592	1.585763	-1.080756
C	-3.266591	-0.516844	-1.438304
C	-2.515563	0.699658	-1.635259
C	-4.382009	-0.526856	-0.399051
H	-4.198825	0.296119	0.308091
H	-5.331682	-0.295365	-0.895938
C	-4.491550	-1.831125	0.386169
H	-4.713604	-2.661515	-0.299319
H	-5.340870	-1.768631	1.073776
C	-3.214056	-2.142619	1.163935
H	-2.994297	-1.288665	1.826359
H	-3.380673	-2.996830	1.833510
C	-2.012985	-2.416713	0.265099
H	-1.085721	-2.534391	0.834507

H	-2.134447	-3.337595	-0.317437
H	-3.481909	-1.100011	-2.339077
C	-0.356342	3.927124	0.792920
C	-0.055971	3.172825	2.070335
H	0.206889	4.863297	0.721511
H	-1.428858	4.165987	0.718319
H	1.014499	3.237113	2.329530
H	-0.634730	3.544115	2.920757
N	-0.446042	1.792561	1.769195
N	0.053063	3.021311	-0.283285
C	-0.245199	0.800257	2.809062
H	-0.579347	-0.182073	2.457177
H	0.809206	0.714109	3.112721
H	-0.838269	1.060163	3.690014
C	-0.194554	3.455066	-1.646536
H	-1.256561	3.660354	-1.840533
H	0.372981	4.368632	-1.848062
H	0.144944	2.692729	-2.352001
H	3.723270	-0.367324	-1.291460
H	3.649455	-1.239096	0.233107
O	0.343859	-2.759332	-2.105203
O	0.976001	-3.541897	-0.100213
C	0.481271	-4.053393	-2.682894
H	-0.106585	-4.042635	-3.601019
H	1.526170	-4.274379	-2.937373
H	0.105114	-4.833975	-2.015640
C	1.709706	-3.441025	1.101117
H	1.412025	-4.287610	1.720949
H	2.795173	-3.501906	0.938172
H	1.483621	-2.513485	1.647934

L36 – Octene (PNCN_S_PCpNMe_X-OMe_TS2)
Electronic Energy: -1505.05792194
Enthalpy: -1504.476221
Free Energy: -1504.565821

24	0.023997	0.804890	0.457132
15	1.721470	-0.845809	-0.105220
7	0.711248	-2.270227	-0.339296
6	-0.632146	-2.105964	-0.392679
7	-1.183157	-0.936989	-0.213675
1	1.090797	-3.198048	-0.487106
6	-2.633803	-1.064760	-0.296366
6	-1.592100	-3.235615	-0.614309
6	-2.910004	-2.496508	-0.814545
1	-3.758242	-2.970617	-0.318731
1	-3.147161	-2.425348	-1.878657
6	-1.625550	2.217287	0.454101
6	-1.052509	2.359191	-0.960669
6	-0.482631	3.727555	-1.304513
6	0.660645	4.194507	-0.413925
6	1.579696	2.151237	0.800076
6	1.810374	3.195653	-0.281873
1	-1.768431	3.206352	0.885389
1	-0.267546	1.607866	-1.264068
1	-1.300856	4.456713	-1.272425
1	1.028461	5.146573	-0.811278
1	2.503887	1.580124	0.976179
1	-2.563678	1.665397	0.426647
1	-1.849403	2.061773	-1.649677
1	-0.139474	3.700838	-2.346843
1	0.277607	4.422153	0.592303
1	1.352055	2.655226	1.751840
1	1.995622	2.712943	-1.256884
1	2.733068	3.753058	-0.063719
6	-0.194314	0.468331	2.470482

1	0.770651	0.644966	2.941293
1	-0.636338	-0.510885	2.649193
6	-1.073389	1.581972	2.321109
1	-0.703457	2.547745	2.653584
1	-2.132031	1.426007	2.506468
1	-1.593848	-3.883486	0.270960
1	-1.299979	-3.863194	-1.460942
6	4.280925	-1.281221	0.175692
6	3.973829	-1.344290	-1.305283
1	4.960917	-2.078258	0.493829
1	4.735499	-0.314232	0.441447
1	3.865031	-2.386875	-1.649530
1	4.749903	-0.867163	-1.910937
7	2.718438	-0.602922	-1.438206
7	2.983729	-1.452637	0.834493
6	2.154860	-0.459227	-2.765543
1	1.923408	-1.427521	-3.234456
1	1.228603	0.124215	-2.718836
1	2.856568	0.077228	-3.410385
6	2.953743	-1.343932	2.282040
1	3.637435	-2.081163	2.712833
1	3.250621	-0.348309	2.643253
1	1.949551	-1.564980	2.652422
8	-3.212801	-0.759032	0.956955
8	-3.055744	-0.067811	-1.170404
6	-3.040711	-1.734719	1.963807
1	-3.342620	-1.274296	2.906218
1	-3.668031	-2.621137	1.799329
1	-1.993762	-2.058029	2.057937
6	-4.465388	0.006034	-1.342613
1	-4.641814	0.800331	-2.069012
1	-4.876493	-0.930538	-1.742950
1	-4.975915	0.247882	-0.405427

L37 – Hexene (PNCN_S_PCpO_X-CF3_Z-CF3-TS1)
Electronic Energy: -2506.53662102
Enthalpy: -2506.137325
Free Energy: -2506.235957

Cr	-1.431990	-0.858426	-0.532245
P	-0.357658	1.189302	0.116404
N	1.298421	0.653316	0.318367
C	1.577328	-0.600200	-0.093207
N	0.636000	-1.460588	-0.380502
H	2.074333	1.281004	0.506075
C	1.221890	-2.659760	-0.973998
C	2.990747	-1.093209	-0.325121
C	2.756865	-2.480475	-0.943916
H	3.230046	-3.260762	-0.348464
H	3.188016	-2.549792	-1.943069
H	-2.795571	-1.766355	-0.410228
H	-2.284880	0.119015	-2.766937
H	-2.912613	1.248818	-1.476561
C	-3.501442	-0.832888	-1.213893
C	-2.682242	0.220816	-1.754992
C	-4.540502	-0.461487	-0.162542
H	-4.279826	0.529136	0.238766
H	-5.511468	-0.344252	-0.657315
C	-4.646345	-1.443611	0.999919
H	-4.973089	-2.426837	0.633691
H	-5.423665	-1.101467	1.689612
C	-3.319506	-1.593568	1.740138
H	-2.973115	-0.599733	2.064607
H	-3.464979	-2.168306	2.663968
C	-2.252763	-2.271609	0.890923
H	-1.276322	-2.307740	1.391036

H	-2.528696	-3.302091	0.647606
H	-3.808769	-1.618181	-1.911481
C	-0.578769	3.697808	0.431191
C	-0.519155	3.058943	1.798953
H	0.072210	4.566346	0.327343
H	-1.599788	3.966652	0.142917
H	0.489221	3.080791	2.227823
H	-1.226286	3.481225	2.512168
O	-0.904255	1.675693	1.571992
O	-0.095859	2.681317	-0.486808
C	3.743905	-0.162746	-1.293116
C	3.743821	-1.201712	1.013927
F	2.972894	0.110993	-2.356363
F	4.868859	-0.730853	-1.725857
F	4.057308	1.006752	-0.706541
F	3.769369	-0.023236	1.659236
F	3.127788	-2.085045	1.810559
F	4.998807	-1.609437	0.821170
C	0.692316	-2.756653	-2.418230
F	1.000155	-3.922990	-2.980941
F	1.197500	-1.769596	-3.167900
F	-0.657970	-2.613293	-2.448389
C	0.814144	-3.920584	-0.182721
F	-0.463659	-4.263104	-0.400741
F	0.974543	-3.709284	1.128983
F	1.582445	-4.958533	-0.539238

L37 – Octene (PNCN_S_PCpO_X-CF3_Z-CF3_TS2)
Electronic Energy: -2585.1447573
Enthalpy: -2584.683241
Free Energy: -2584.787528

Cr	-1.442457	-0.714849	0.345944
P	-0.142688	1.263567	-0.053419
N	1.493753	0.67368	-0.014643
C	1.700834	-0.64544	-0.218200
N	0.723700	-1.499495	-0.318917
H	2.301392	1.274961	0.102493
C	1.271336	-2.808473	-0.656598
C	3.100886	-1.232976	-0.269157
C	2.814075	-2.709887	-0.583068
H	3.214649	-3.363257	0.192974
H	3.278968	-3.020083	-1.519527
C	-2.863467	-2.291615	0.901017
C	-3.006846	-2.179556	-0.620037
C	-4.412216	-1.797938	-1.084057
C	-4.974237	-0.516314	-0.476913
C	-2.997785	0.625559	0.685412
C	-4.017317	0.673044	-0.444460
H	-3.751863	-1.901262	1.393238
H	-2.334881	-1.444120	-1.152533
H	-5.084939	-2.634029	-0.864762
H	-5.873784	-0.251290	-1.041722
H	-2.586207	1.624361	0.879991
H	-2.697906	-3.325348	1.186946
H	-2.675124	-3.114822	-1.075678
H	-4.384845	-1.706854	-2.176467
H	-5.322227	-0.704241	0.548040
H	-3.465778	0.306526	1.627627
H	-3.515773	0.782229	-1.421211
H	-4.617758	1.587467	-0.338308
C	-0.746231	-0.569828	2.283135
H	-1.072667	0.360231	2.744978
H	0.32972	-0.744569	2.286136
C	-1.586627	-1.717056	2.413336
H	-2.464649	-1.629800	3.045029

H	-1.095423	-2.682409	2.476023
C	-0.181065	3.751912	0.443628
C	0.231696	3.562902	-0.998549
H	0.459479	4.445874	0.988878
H	-1.225294	4.066025	0.535418
H	1.32029	3.582397	-1.130189
H	-0.225668	4.277036	-1.682595
O	-0.261521	2.243692	-1.349071
O	-0.038474	2.447397	1.062721
C	3.978957	-0.573458	-1.345311
F	5.171602	-1.167529	-1.414239
F	4.17679	0.735303	-1.091627
F	3.392138	-0.664077	-2.543895
C	3.753203	-1.085332	1.120549
F	4.903149	-1.755613	1.188470
F	2.924687	-1.574340	2.058162
F	3.992943	0.200700	1.425705
C	0.824878	-3.155372	-2.091021
F	1.266615	-4.364611	-2.453944
F	1.321371	-2.251653	-2.947217
F	-0.510308	-3.136664	-2.221634
C	0.752637	-3.856725	0.336455
F	-0.580222	-4.011429	0.243460
F	1.027756	-3.472867	1.593985
F	1.32461	-5.046359	0.131988

L38 – Hexene (PNCN_S_PCpO_X-CH3_Z-CH3-TS1)
Electronic Energy: -1315.79340236
Enthalpy: -1315.309908
Free Energy: -1315.389540

Cr	-1.413755	-0.646330	-0.332554
P	-0.207606	1.331453	0.308792
N	1.417843	0.783432	0.219839
C	1.601017	-0.517307	-0.164988
N	0.596339	-1.334251	-0.285491
H	2.223365	1.398989	0.229528
C	1.084319	-2.654315	-0.797527
C	2.965001	-1.077933	-0.490412
C	2.541371	-2.365475	-1.221054
H	3.207669	-3.203126	-0.997378
H	2.582830	-2.197450	-2.303189
H	-2.719999	-1.612811	-0.543516
H	-2.198027	0.916180	-2.296285
H	-3.011006	1.526878	-0.782778
C	-3.405341	-0.566491	-1.224618
C	-2.655301	0.659200	-1.339848
C	-4.617487	-0.602386	-0.299817
H	-4.549584	0.252556	0.387352
H	-5.519365	-0.438539	-0.901012
C	-4.748102	-1.881369	0.522757
H	-4.872641	-2.746428	-0.144322
H	-5.658675	-1.829636	1.127245
C	-3.535276	-2.101555	1.423887
H	-3.387875	-1.202405	2.042607
H	-3.729109	-2.917206	2.131862
C	-2.258216	-2.396058	0.644709
H	-1.379714	-2.395233	1.302796
H	-2.299000	-3.373278	0.149497
H	-3.520122	-1.145923	-2.146410
C	-0.414845	3.856235	0.502153
C	-0.103063	3.307701	1.875336
H	0.184026	4.728490	0.236448
H	-1.477692	4.095593	0.388205
H	0.965419	3.366807	2.114992
H	-0.677666	3.774037	2.675473

O	-0.496856	1.915180	1.807945
O	-0.073514	2.793962	-0.418596
C	3.782863	-0.144870	-1.380091
H	4.692746	-0.655437	-1.707425
H	3.233034	0.159556	-2.275614
H	4.104565	0.758066	-0.849420
C	3.733015	-1.347773	0.809513
H	4.707094	-1.787103	0.576748
H	3.911911	-0.422202	1.366536
H	3.203137	-2.038073	1.471042
C	0.212287	-3.054640	-1.977587
H	0.585356	-3.972451	-2.441990
H	-0.819407	-3.245676	-1.661438
H	0.203613	-2.272513	-2.745449
C	1.004462	-3.709294	0.299953
H	-0.028464	-3.908052	0.594744
H	1.429067	-4.651304	-0.059486
H	1.560788	-3.412059	1.193453

L38 – Octene (PNCN_S_PCpO_X-CH3_Z-CH3-TS2)
Electronic Energy: -1394.4007084
Enthalpy: -1393.854956
Free Energy: -1393.938693

Cr	-1.370700	-0.643559	0.302295
P	-0.027872	1.329180	0.039205
N	1.541295	0.700677	-0.191274
Cr	1.685894	-0.656815	-0.338250
N	0.680028	-1.471006	-0.276305
H	2.374874	1.273849	-0.255780
C	1.186145	-2.871950	-0.411770
C	3.059096	-1.266756	-0.506982
C	2.659834	-2.710191	-0.848649
H	3.311562	-3.445702	-0.368011
H	2.740876	-2.865276	-1.930111
C	-2.552786	-2.460813	0.403518
C	-2.801180	-1.967903	-1.035244
C	-4.248246	-1.627036	-1.363347
C	-4.872233	-0.542935	-0.497384
C	-2.958871	0.677994	0.659234
C	-4.048704	0.739028	-0.399591
H	-3.507451	-2.732538	0.849522
H	-2.177272	-1.099864	-1.398849
H	-4.837467	-2.548421	-1.290218
H	-5.867347	-0.324836	-0.898942
H	-2.555130	1.684343	0.839905
H	-1.900884	-3.334671	0.396134
H	-2.429246	-2.748939	-1.707442
H	-4.291185	-1.320841	-2.415845
H	-5.042670	-0.927964	0.519171
H	-3.396650	0.366203	1.618255
H	-3.626189	0.989189	-1.386660
H	-4.728378	1.571047	-0.165962
C	-0.977345	-0.754272	2.310470
H	-1.256041	0.197483	2.758966
H	0.049886	-1.073908	2.485121
C	-1.987643	-1.762879	2.214872
H	-2.983669	-1.488352	2.550133
H	-1.715324	-2.783031	2.471786
C	-0.072316	3.761737	0.775691
C	0.159011	3.728368	-0.718189
H	0.600803	4.441016	1.300692
H	-1.109078	4.010594	1.026426
H	1.222389	3.817029	-0.974624
H	-0.405814	4.483014	-1.265370
O	-0.324005	2.429082	-1.135214

O	0.211352	2.420926	1.236372
C	0.385262	-3.612527	-1.471282
C	1.059164	-3.569297	0.938105
H	0.841100	-4.586196	-1.674981
H	1.387614	-4.610395	0.864537
H	0.359486	-3.050463	-2.410324
H	-0.643458	-3.799092	-1.150949
H	0.020979	-3.573652	1.286064
H	1.665078	-3.080966	1.707446
C	3.862204	-0.599488	-1.620943
H	4.135244	0.432148	-1.371235
H	4.797966	-1.142931	-1.778882
H	3.317589	-0.589281	-2.569689
C	3.828403	-1.152831	0.815140
H	4.809310	-1.625636	0.713453
H	3.994279	-0.106861	1.094781
H	3.305912	-1.641827	1.642532

L39 – Hexene (PNCN_S_PCpO_X-F_TS1)
Electronic Energy: -1357.00809873
Enthalpy: -1356.656088
Free Energy: -1356.728027

Cr	-1.450090	-0.589065	-0.327097
P	-0.215012	1.375729	0.324654
N	1.427220	0.853628	0.085853
C	1.602674	-0.440537	-0.262400
N	0.576515	-1.250781	-0.354453
H	2.233780	1.467821	0.092835
C	1.064065	-2.544627	-0.762972
C	2.924137	-1.059915	-0.582019
C	2.495267	-2.367911	-1.243597
H	3.109107	-3.228035	-0.979741
H	2.483437	-2.269163	-2.330484
H	-2.684272	-1.569205	-0.783008
H	-2.284012	1.148995	-2.139999
H	-3.076668	1.588013	-0.556749
C	-3.440573	-0.457171	-1.202285
C	-2.715571	0.788528	-1.205496
C	-4.584754	-0.626495	-0.207954
H	-4.481963	0.147686	0.566144
H	-5.529860	-0.418528	-0.722750
C	-4.636404	-1.990732	0.474137
H	-4.835319	-2.776656	-0.267690
H	-5.478380	-2.009708	1.172541
C	-3.336719	-2.311697	1.207595
H	-3.099643	-1.481640	1.896098
H	-3.466682	-3.190314	1.852465
C	-2.171033	-2.543297	0.257116
H	-1.233258	-2.746450	0.784300
H	-2.350163	-3.386349	-0.418411
H	-3.612494	-0.915895	-2.180785
H	3.539594	-0.416156	-1.214993
H	3.479867	-1.222307	0.348463
C	-0.425954	3.893618	0.544341
C	0.021718	3.348014	1.880487
H	0.134439	4.772829	0.224451
H	-1.497444	4.118996	0.530486
H	1.105794	3.425416	2.022283
H	-0.486918	3.800153	2.731555
O	-0.350244	1.945872	1.846022
O	-0.160727	2.835168	-0.408650
F	0.235152	-3.050181	-1.715333
F	0.986931	-3.404388	0.296633

L39 – Octene (PNCN_S_PCpO_X-F_TS2)

Electronic Energy: -1435.61926373
Enthalpy: -1435.205785
Free Energy: -1435.283250

Cr	-1.376810	-0.544886	0.285647
P	-0.009912	1.440314	0.062868
N	1.574702	0.779749	-0.189838
C	1.690149	-0.561218	-0.343888
N	0.642629	-1.338415	-0.284142
H	2.420047	1.338451	-0.226253
C	1.085489	-2.697160	-0.399463
C	2.998070	-1.259210	-0.546586
C	2.555381	-2.698474	-0.796759
H	3.110196	-3.436931	-0.219254
H	2.630211	-2.962590	-1.852444
C	-2.313718	-2.482825	0.319545
C	-2.621043	-1.978088	-1.099953
C	-4.098536	-1.783697	-1.406581
C	-4.809437	-0.781461	-0.507880
C	-3.033380	0.664114	0.619077
C	-4.131149	0.586145	-0.430825
H	-3.221904	-2.897097	0.752417
H	-2.104907	-1.029593	-1.429772
H	-4.591013	-2.760785	-1.341013
H	-5.837067	-0.674416	-0.870052
H	-2.696235	1.704584	0.735673
H	-1.535475	-3.243502	0.296395
H	-2.155144	-2.686658	-1.792133
H	-4.190861	-1.464333	-2.451911
H	-4.896155	-1.190470	0.510010
H	-3.435395	0.369803	1.599577
H	-3.742888	0.864493	-1.424103
H	-4.895637	1.343296	-0.205658
C	-0.968636	-0.656564	2.295952
H	-1.338121	0.260254	2.751681
H	0.078521	-0.889840	2.484678
C	-1.876599	-1.751714	2.168147
H	-2.903205	-1.581092	2.479606
H	-1.506176	-2.745818	2.399286
H	3.613976	-1.151018	0.352595
H	3.565691	-0.819355	-1.370935
C	0.064875	3.864649	0.813288
C	0.286655	3.829360	-0.682041
H	0.775737	4.502492	1.339898
H	-0.956024	4.163410	1.071655
H	1.349888	3.871905	-0.948583
H	-0.249160	4.609468	-1.222002
O	-0.256962	2.553164	-1.103879
O	0.277724	2.504945	1.267451
F	0.869140	-3.327805	0.799758
F	0.298420	-3.359853	-1.295359

L40 – Hexene (PNCN_S_PCpO_X-F_Z-F-TS1)
Electronic Energy: -1555.44446734
Enthalpy: -1555.107529
Free Energy: -1555.185110

Cr	-1.466271	-0.586434	-0.307726
P	-0.228880	1.394409	0.340935
N	1.423926	0.847635	0.125444
C	1.567956	-0.437396	-0.230210
N	0.561712	-1.260163	-0.344430
H	2.245284	1.444985	0.105325
C	1.056626	-2.541419	-0.803979
C	2.906113	-1.083485	-0.554169
C	2.493375	-2.349503	-1.269985

H	3.129535	-3.198853	-1.026917
H	2.502834	-2.175213	-2.346696
H	-2.688722	-1.580548	-0.752770
H	-2.300726	1.143193	-2.124526
H	-3.111521	1.571707	-0.546672
C	-3.451194	-0.475096	-1.201138
C	-2.739729	0.777239	-1.195683
C	-4.611483	-0.660020	-0.229151
H	-4.537818	0.116519	0.545559
H	-5.547709	-0.467137	-0.765409
C	-4.657142	-2.024524	0.452536
H	-4.819858	-2.814848	-0.293311
H	-5.517344	-2.059195	1.127362
C	-3.372678	-2.316981	1.223390
H	-3.171556	-1.480573	1.914983
H	-3.501833	-3.196669	1.866699
C	-2.175248	-2.529286	0.309254
H	-1.245542	-2.684619	0.868293
H	-2.303650	-3.391841	-0.352980
H	-3.595001	-0.941428	-2.180559
C	-0.357068	3.919358	0.528700
C	0.076957	3.369673	1.867461
H	0.241677	4.765925	0.191572
H	-1.417134	4.192128	0.518723
H	1.164516	3.396406	2.001177
H	-0.405314	3.851914	2.717040
O	-0.357854	1.982428	1.851132
O	-0.153528	2.835735	-0.415909
F	0.238334	-2.985517	-1.791190
F	0.966239	-3.441771	0.208327
F	3.682608	-0.248765	-1.285782
F	3.564054	-1.327927	0.610523

L40 – Octene (PNCN_S_PCpO_X-F_Z-F-TS2)
Electronic Energy: -1634.05642413
Enthalpy: -1633.657675
Free Energy: -1633.738834

Cr	-1.396869	-0.546035	0.244904
P	-0.029334	1.454281	0.017988
N	1.561593	0.785494	-0.254755
C	1.659638	-0.549540	-0.373873
N	0.639027	-1.354030	-0.339416
H	2.422698	1.324373	-0.271321
C	1.119513	-2.711442	-0.403531
C	2.999369	-1.264617	-0.457795
C	2.602635	-2.693638	-0.749800
H	3.172160	-3.412150	-0.162695
H	2.731496	-2.903042	-1.811974
C	-2.322161	-2.487049	0.280924
C	-2.665176	-1.975012	-1.127497
C	-4.150586	-1.780949	-1.393836
C	-4.839172	-0.790290	-0.465681
C	-3.041480	0.663436	0.618426
C	-4.166093	0.580343	-0.401029
H	-3.215419	-2.916645	0.729556
H	-2.155521	-1.025788	-1.465585
H	-4.638457	-2.760030	-1.325060
H	-5.877826	-0.685979	-0.795263
H	-2.698175	1.703556	0.718754
H	-1.535277	-3.238536	0.238862
H	-2.219031	-2.680653	-1.836082
H	-4.271736	-1.451036	-2.432780
H	-4.892936	-1.207450	0.551109
H	-3.414053	0.374152	1.611746
H	-3.807044	0.865293	-1.403113

H	-4.926868	1.333078	-0.150364
C	-0.946197	-0.675417	2.246026
H	-1.299755	0.242592	2.712001
H	0.101220	-0.920282	2.418323
C	-1.865279	-1.762110	2.130573
H	-2.887236	-1.584763	2.453388
H	-1.500294	-2.760121	2.353264
C	0.095895	3.863005	0.807908
C	0.308214	3.844877	-0.689370
H	0.829450	4.469339	1.340211
H	-0.913758	4.186603	1.079050
H	1.369262	3.868316	-0.964577
H	-0.216780	4.641898	-1.214639
O	-0.264160	2.584133	-1.128182
O	0.267301	2.488369	1.241592
F	0.882381	-3.306877	0.802133
F	0.381424	-3.402017	-1.310462
F	3.799415	-0.699588	-1.394356
F	3.626614	-1.119639	0.742724

L41 – Hexene (PNCN_S_PCpO_X-H_TS1)
Electronic Energy: -1158.49112427
Enthalpy: -1158.124359
Free Energy: -1158.194398

Cr	-1.438442	-0.525556	-0.351239
P	-0.180739	1.417015	0.282308
N	1.436903	0.863883	0.047428
C	1.580209	-0.450641	-0.294525
N	0.543513	-1.230097	-0.424508
H	2.254517	1.460067	0.033488
C	1.018137	-2.592494	-0.733270
C	2.900158	-1.113876	-0.515041
C	2.472463	-2.422716	-1.181259
H	3.101555	-3.269623	-0.905726
H	2.519341	-2.317901	-2.268544
H	0.378029	-3.046071	-1.494424
H	-2.688055	-1.495745	-0.757651
H	-2.405174	1.337806	-1.985138
H	-3.120560	1.618683	-0.330640
C	-3.470665	-0.371595	-1.124693
C	-2.775524	0.888102	-1.063954
C	-4.591435	-0.645859	-0.127228
H	-4.475993	0.046231	0.719030
H	-5.546246	-0.390017	-0.600232
C	-4.622055	-2.074663	0.407988
H	-4.797566	-2.781944	-0.414732
H	-5.471070	-2.185605	1.088362
C	-3.325965	-2.439836	1.127918
H	-3.133711	-1.691375	1.914069
H	-3.438954	-3.393468	1.658316
C	-2.124774	-2.516448	0.191825
H	-1.193412	-2.686189	0.744735
H	-2.225014	-3.331443	-0.534524
H	-3.649036	-0.768542	-2.129070
H	0.930983	-3.210338	0.169797
H	3.585430	-0.505248	-1.111740
H	3.382772	-1.270190	0.458707
C	-0.389521	3.938736	0.454862
C	0.035858	3.414833	1.810203
H	0.174800	4.813194	0.128775
H	-1.460969	4.163256	0.418179
H	1.118081	3.496650	1.966647
H	-0.485212	3.879078	2.647005
O	-0.334061	2.014615	1.792134
O	-0.102569	2.867239	-0.470751

L41 – Octene (PNCN_S_PCpO_X-H_TS2)
Electronic Energy: -1237.10090288
Enthalpy: -1236.673017
Free Energy: -1236.747339

Cr	-1.363081	-0.507070	0.260958
P	0.015162	1.454771	0.043300
N	1.576437	0.761156	-0.169766
C	1.660037	-0.596335	-0.332000
N	0.605212	-1.352567	-0.301956
H	2.435005	1.296039	-0.197479
C	1.037762	-2.753435	-0.416530
C	2.961448	-1.316218	-0.496419
C	2.484670	-2.706149	-0.920018
H	3.099404	-3.512500	-0.518722
H	2.503858	-2.790169	-2.009789
H	0.370418	-3.300900	-1.089843
C	-2.267911	-2.469126	0.349847
C	-2.591115	-2.002881	-1.080726
C	-4.076769	-1.843768	-1.373436
C	-4.789287	-0.830205	-0.488399
C	-3.023064	0.715307	0.523622
C	-4.148233	0.557326	-0.489107
H	-3.163935	-2.908193	0.783744
H	-2.095019	-1.051504	-1.432521
H	-4.549573	-2.827832	-1.276730
H	-5.829767	-0.767213	-0.821537
H	-2.697851	1.765343	0.556666
H	-1.470421	-3.212280	0.344047
H	-2.123838	-2.718408	-1.766792
H	-4.190868	-1.552130	-2.424349
H	-4.835288	-1.202176	0.546457
H	-3.401520	0.491412	1.532164
H	-3.797807	0.800777	-1.504670
H	-4.926116	1.302980	-0.274699
C	-0.956180	-0.579338	2.271097
H	-1.322215	0.347844	2.706838
H	0.090546	-0.808784	2.467866
C	-1.872422	-1.673219	2.170213
H	-2.901383	-1.480711	2.462452
H	-1.520569	-2.660485	2.455610
H	0.956399	-3.227361	0.572775
H	3.488363	-1.322526	0.466822
H	3.625921	-0.829236	-1.215769
C	0.039200	3.855428	0.870636
C	0.311635	3.872828	-0.619270
H	0.716035	4.490759	1.443288
H	-0.996639	4.124353	1.102538
H	1.382830	3.947234	-0.844261
H	-0.221735	4.657572	-1.155134
O	-0.186992	2.602609	-1.098823
O	0.269318	2.490095	1.283844

L42 – Hexene (PNCN_S_PCpO_X-H_Z-CF3-TS1)
Electronic Energy: -1832.53731323
Enthalpy: -1832.153832
Free Energy: -1832.237608

Cr	-1.454260	-0.501372	-0.350779
P	-0.175858	1.449261	0.286223
N	1.444934	0.875616	0.081731
C	1.574953	-0.435346	-0.251467
N	0.553752	-1.224901	-0.396609
H	2.279807	1.447919	0.141918
C	1.021674	-2.584473	-0.697580

C	2.921925	-1.102596	-0.463270
C	2.495903	-2.445466	-1.079447
H	3.114657	-3.271807	-0.726970
H	2.605578	-2.391663	-2.164555
H	-2.725576	-1.444297	-0.757010
H	-2.491717	1.454220	-1.834103
H	-3.148412	1.614396	-0.137487
C	-3.511621	-0.320578	-1.061339
C	-2.827345	0.939919	-0.933531
C	-4.620339	-0.667505	-0.074217
H	-4.492635	-0.043168	0.821388
H	-5.579927	-0.374827	-0.515403
C	-4.647738	-2.133369	0.348010
H	-4.822368	-2.773663	-0.528221
H	-5.495409	-2.299240	1.019424
C	-3.350664	-2.550075	1.036178
H	-3.172088	-1.876091	1.889152
H	-3.456793	-3.551330	1.472835
C	-2.139409	-2.525015	0.110305
H	-1.216037	-2.708884	0.671485
H	-2.205262	-3.292324	-0.670555
H	-3.698130	-0.656255	-2.086470
C	-0.321290	3.979267	0.384255
C	0.116467	3.481982	1.741916
H	0.265914	4.823693	0.021529
H	-1.385348	4.237294	0.362625
H	1.204393	3.523293	1.870747
H	-0.367347	3.991831	2.574510
O	-0.308580	2.092671	1.776597
O	-0.093753	2.869159	-0.517509
H	0.416782	-3.016112	-1.498432
H	0.884949	-3.211300	0.190467
C	3.811058	-0.306074	-1.421507
C	3.604185	-1.305183	0.897685
F	3.122419	-0.005084	-2.536180
F	4.891027	-1.002741	-1.773974
F	4.220838	0.858223	-0.875618
F	3.800230	-0.141013	1.537822
F	2.814619	-2.067869	1.676358
F	4.783370	-1.917427	0.770853

L42 – Octene (PNCN_S_PCpO_X-H_Z-CF3_TS2)
Electronic Energy: -1911.14650595
Enthalpy: -1910.701710
Free Energy: -1910.791533

Cr	-1.381266	-0.504367	0.239519
P	-0.012387	1.474293	0.047942
N	1.560031	0.784033	-0.146538
C	1.649169	-0.565108	-0.315490
N	0.616758	-1.344464	-0.308705
H	2.418854	1.322151	-0.126123
C	1.051894	-2.737774	-0.415858
C	2.983777	-1.280393	-0.444110
C	2.526123	-2.697952	-0.825851
H	3.131811	-3.466388	-0.343611
H	2.625667	-2.830058	-1.905105
C	-2.273333	-2.467263	0.276338
C	-2.618611	-1.957604	-1.134532
C	-4.108199	-1.798410	-1.404691
C	-4.821256	-0.828269	-0.473158
C	-3.055401	0.668445	0.608800
C	-4.184048	0.559271	-0.405283
H	-3.164397	-2.907823	0.719206
H	-2.133988	-0.993665	-1.466407
H	-4.572739	-2.789233	-1.341652

H	-5.862321	-0.751100	-0.802793
H	-2.734990	1.716340	0.703299
H	-1.485699	-3.219566	0.232989
H	-2.158666	-2.649174	-1.848922
H	-4.234032	-1.466183	-2.442283
H	-4.864062	-1.250007	0.542316
H	-3.421773	0.378173	1.604788
H	-3.837002	0.854857	-1.408511
H	-4.964788	1.290122	-0.151241
C	-0.917625	-0.639923	2.237731
H	-1.288126	0.265852	2.714251
H	0.137661	-0.860135	2.400861
C	-1.819251	-1.742280	2.116866
H	-2.841337	-1.580250	2.447392
H	-1.443542	-2.735180	2.346871
C	0.086484	3.892428	0.813796
C	0.356641	3.857435	-0.673692
H	0.796281	4.508747	1.366769
H	-0.934240	4.216462	1.040097
H	1.428354	3.872792	-0.905949
H	-0.142106	4.652284	-1.227415
O	-0.205228	2.596307	-1.118883
O	0.247573	2.525561	1.268674
H	0.432644	-3.268789	-1.144616
H	0.905701	-3.226829	0.555784
C	3.861656	-0.660323	-1.531347
F	4.927622	-1.417836	-1.791138
F	4.296127	0.570008	-1.185399
F	3.149319	-0.529372	-2.664298
C	3.688720	-1.282792	0.919029
F	4.844567	-1.947351	0.869798
F	2.892430	-1.888928	1.822956
F	3.936027	-0.041545	1.368374

L43 – Hexene (PNCN_S_PCpO_X-H_Z-CH3-TS1)
Electronic Energy: -1237.16687435
Enthalpy: -1236.741225
Free Energy: -1236.815231

Cr	-1.452141	-0.503376	-0.372790
P	-0.169302	1.450602	0.252328
N	1.441195	0.880323	0.051837
C	1.577919	-0.435033	-0.284878
N	0.539541	-1.208496	-0.431351
H	2.269917	1.464561	0.056424
C	1.020542	-2.564878	-0.755815
C	2.921610	-1.101120	-0.470390
C	2.464966	-2.372406	-1.208040
H	3.100843	-3.233213	-0.988704
H	2.497442	-2.200121	-2.289297
H	-2.726390	-1.456567	-0.752541
H	-2.525298	1.424201	-1.870629
H	-3.144104	1.617646	-0.163840
C	-3.525398	-0.335715	-1.039296
C	-2.838082	0.927383	-0.952055
C	-4.598384	-0.668353	-0.009059
H	-4.429634	-0.043408	0.879632
H	-5.572872	-0.368202	-0.411440
C	-4.621389	-2.133192	0.417126
H	-4.829283	-2.772737	-0.452496
H	-5.447695	-2.292691	1.116461
C	-3.305220	-2.559560	1.062180
H	-3.097268	-1.888684	1.911196
H	-3.404784	-3.561350	1.499631
C	-2.122388	-2.536480	0.099449
H	-1.183570	-2.733354	0.628323

H	-2.219132	-3.299641	-0.682501
H	-3.748852	-0.686721	-2.051848
C	-0.354650	3.981420	0.325743
C	0.083043	3.505776	1.691288
H	0.215545	4.837165	-0.038495
H	-1.423841	4.217762	0.295442
H	1.169721	3.570646	1.823952
H	-0.413222	4.017429	2.515651
O	-0.316640	2.112278	1.738173
O	-0.093087	2.870746	-0.561539
H	0.378500	-3.014573	-1.517457
H	0.945573	-3.195130	0.140128
C	3.904899	-0.253609	-1.265755
H	4.205264	0.646485	-0.717559
H	4.818192	-0.823274	-1.457627
H	3.495060	0.053524	-2.232492
C	3.496754	-1.425948	0.914428
H	4.453129	-1.944049	0.802247
H	3.676106	-0.518122	1.498992
H	2.829876	-2.072205	1.493490

L43 – Octene (PNCN_S_PCpO_X-H_Z-CH3-TS2)
Electronic Energy: -1315.77453223
Enthalpy: -1315.287534
Free Energy: -1315.366984

Cr	-1.362206	-0.522587	0.284780
P	0.012954	1.451292	0.030885
N	1.563502	0.761778	-0.224934
C	1.650679	-0.597316	-0.366991
N	0.602055	-1.358581	-0.291399
H	2.418474	1.302398	-0.297028
C	1.043223	-2.757312	-0.397445
C	2.977761	-1.311193	-0.511903
C	2.466146	-2.695194	-0.949416
H	3.102060	-3.507927	-0.590652
H	2.443417	-2.748970	-2.043080
C	-2.287703	-2.470949	0.309707
C	-2.616973	-1.955626	-1.102310
C	-4.102610	-1.776856	-1.382168
C	-4.807870	-0.792219	-0.459500
C	-3.029252	0.674380	0.638289
C	-4.149142	0.585468	-0.387933
H	-3.187071	-2.902338	0.744870
H	-2.120337	-0.996683	-1.428457
H	-4.582482	-2.760431	-1.318295
H	-5.845130	-0.699881	-0.797733
H	-2.696116	1.717727	0.740063
H	-1.506598	-3.230522	0.272459
H	-2.160162	-2.651528	-1.814646
H	-4.217394	-1.446733	-2.421858
H	-4.865229	-1.210483	0.556821
H	-3.414053	0.388886	1.628896
H	-3.785061	0.872503	-1.387926
H	-4.921844	1.329094	-0.145929
C	-0.939730	-0.656266	2.291229
H	-1.308823	0.256591	2.754885
H	0.110112	-0.885128	2.472941
C	-1.849149	-1.749590	2.158480
H	-2.874974	-1.577709	2.472167
H	-1.486717	-2.746671	2.392233
C	0.088891	3.886600	0.750396
C	0.296294	3.833031	-0.746278
H	0.800582	4.536592	1.261163
H	-0.931508	4.184217	1.013519
H	1.357886	3.870938	-1.020806

H	-0.242062	4.608513	-1.290717
O	-0.253029	2.554201	-1.146000
O	0.315505	2.536115	1.218292
C	3.910730	-0.659077	-1.523075
H	4.256255	0.324730	-1.185295
H	4.803673	-1.275808	-1.658135
H	3.438235	-0.537718	-2.502210
C	3.645274	-1.367194	0.868919
H	4.589953	-1.913799	0.801338
H	3.868128	-0.365944	1.251559
H	3.016505	-1.875148	1.607486
H	0.998714	-3.218495	0.600329
H	0.359084	-3.319975	-1.040021

L44 – Hexene (PNCN_S_PCpO_X-H_Z-F-TS1)
Electronic Energy: -1356.98558929
Enthalpy: -1356.633446
Free Energy: -1356.705442

Cr	-1.467552	-0.511886	-0.373699
P	-0.183458	1.447487	0.266964
N	1.435634	0.863908	0.086218
C	1.549874	-0.443490	-0.248289
N	0.537107	-1.235817	-0.425727
H	2.278381	1.429800	0.092304
C	1.039184	-2.588785	-0.746535
C	2.885132	-1.141069	-0.402804
C	2.509128	-2.408905	-1.126315
H	3.149326	-3.243485	-0.841243
H	2.614128	-2.234143	-2.199715
H	-2.743796	-1.453483	-0.770126
H	-2.522337	1.432795	-1.860994
H	-3.146717	1.617115	-0.154850
C	-3.537164	-0.326655	-1.048122
C	-2.843433	0.931124	-0.947963
C	-4.614530	-0.663893	-0.024082
H	-4.448400	-0.045228	0.869312
H	-5.585898	-0.358377	-0.429534
C	-4.643557	-2.131620	0.391592
H	-4.852411	-2.764620	-0.482435
H	-5.471275	-2.292704	1.088604
C	-3.330201	-2.566590	1.036278
H	-3.120464	-1.902877	1.890352
H	-3.432682	-3.571148	1.466245
C	-2.146388	-2.542611	0.075485
H	-1.209065	-2.746369	0.605030
H	-2.245142	-3.298250	-0.713380
H	-3.756642	-0.668881	-2.064507
C	-0.321113	3.979130	0.342225
C	0.100058	3.490204	1.708121
H	0.274402	4.817451	-0.021177
H	-1.383442	4.242615	0.307612
H	1.187019	3.524799	1.846762
H	-0.388067	4.010049	2.532005
O	-0.334955	2.104424	1.749523
O	-0.090728	2.860483	-0.548469
F	3.790234	-0.356654	-1.042392
F	3.382602	-1.379172	0.848645
H	0.436750	-3.022848	-1.546992
H	0.923601	-3.227992	0.135926

L44 – Octene (PNCN_S_PCpO_X-H_Z-F-TS2)
Electronic Energy: -1435.59384849
Enthalpy: -1435.180415
Free Energy: -1435.258531

Cr	-1.381413	-0.516588	0.294500
P	-0.002361	1.466522	0.070850
N	1.557693	0.771532	-0.175872
C	1.631059	-0.577561	-0.320477
N	0.614768	-1.374095	-0.245974
H	2.421631	1.299033	-0.251840
C	1.085367	-2.764457	-0.373401
C	2.952453	-1.296254	-0.498375
C	2.522487	-2.687695	-0.893408
H	3.188685	-3.445760	-0.481816
H	2.544208	-2.756876	-1.983228
C	-2.288862	-2.470770	0.320396
C	-2.598807	-1.967514	-1.100264
C	-4.080804	-1.805847	-1.407309
C	-4.808731	-0.819618	-0.504474
C	-3.057747	0.671488	0.606267
C	-4.160697	0.563081	-0.435838
H	-3.189705	-2.912817	0.741265
H	-2.108070	-1.002807	-1.420838
H	-4.552023	-2.793394	-1.342813
H	-5.840850	-0.737590	-0.860029
H	-2.728901	1.717108	0.698018
H	-1.496923	-3.219988	0.302295
H	-2.121537	-2.660956	-1.801409
H	-4.180558	-1.485601	-2.451484
H	-4.879114	-1.229589	0.514339
H	-3.453890	0.395800	1.594741
H	-3.785074	0.845001	-1.432727
H	-4.940787	1.303705	-0.209668
C	-0.992073	-0.632493	2.308071
H	-1.372167	0.284308	2.754786
H	0.053973	-0.856723	2.513439
C	-1.895631	-1.730209	2.170571
H	-2.928195	-1.559086	2.462014
H	-1.533339	-2.722930	2.422112
C	0.102698	3.894071	0.806247
C	0.328115	3.843681	-0.688186
H	0.825209	4.520810	1.330239
H	-0.912729	4.214966	1.059539
H	1.392510	3.863238	-0.951847
H	-0.191490	4.629531	-1.235556
O	-0.238814	2.574421	-1.102233
O	0.285326	2.533466	1.271595
F	3.749120	-0.664543	-1.400210
F	3.618180	-1.268435	0.696271
H	0.423637	-3.319329	-1.043908
H	1.028205	-3.243166	0.612441

L45 – Hexene (PNCN_S_PCpO_X-H_Z-OMe-TS1)
Electronic Energy: -1387.55812822
Enthalpy: -1387.121675
Free Energy: -1387.201180

Cr	-1.362996	-0.496789	-0.281869
P	-0.187544	1.412870	0.628391
N	1.442718	0.871840	0.463681
C	1.607883	-0.421379	0.081722
N	0.613154	-1.228176	-0.138065
H	2.279806	1.400203	0.687946
C	1.155778	-2.541133	-0.542558
C	2.967709	-1.024626	-0.224883
C	2.631981	-2.510135	-0.150840
H	2.762380	-2.852821	0.879899
H	3.269009	-3.102438	-0.808838
H	-2.553408	-1.452407	-0.863817
H	-2.069812	1.391668	-2.004668

H	-3.008473	1.666926	-0.464289
C	-3.267915	-0.312321	-1.330581
C	-2.577269	0.938500	-1.152744
C	-4.518601	-0.593675	-0.505745
H	-4.516471	0.079849	0.363217
H	-5.397934	-0.320338	-1.100647
C	-4.634930	-2.032958	-0.010660
H	-4.694071	-2.720454	-0.866402
H	-5.574324	-2.149774	0.538120
C	-3.459752	-2.428974	0.880835
H	-3.383837	-1.703428	1.706711
H	-3.655387	-3.396348	1.360895
C	-2.132804	-2.486598	0.132770
H	-1.292602	-2.648005	0.819492
H	-2.112991	-3.294591	-0.608105
H	-3.302395	-0.698555	-2.354002
C	-0.378445	3.914865	1.017467
C	-0.040758	3.261295	2.337446
H	0.223801	4.799440	0.805752
H	-1.440962	4.170893	0.945876
H	1.032426	3.298083	2.559141
H	-0.597600	3.665376	3.182512
O	-0.441230	1.877140	2.172726
O	-0.069175	2.923894	0.010230
O	3.321561	-0.769491	-1.569424
O	3.880859	-0.506841	0.686327
C	3.601788	0.587772	-1.891730
H	4.081549	0.574367	-2.870713
H	2.688640	1.193995	-1.959996
H	4.286799	1.044548	-1.168494
C	5.174868	-1.101588	0.597539
H	5.573135	-1.047016	-0.421175
H	5.821436	-0.539786	1.271129
H	5.150434	-2.149950	0.918528
H	0.596405	-3.337438	-0.045507
H	1.021212	-2.666588	-1.622902

L45 – Octene (PNCN_S_PCpO_X-H_Z-OMe-TS2)
Electronic Energy: -1466.166716
Enthalpy: -1465.669289
Free Energy: -1465.753535

24	-1.298963	-0.550848	0.129974
15	0.090060	1.404659	-0.242117
7	1.595994	0.669115	-0.621133
6	1.629824	-0.688527	-0.721841
7	0.580982	-1.443396	-0.644164
1	2.471042	1.158022	-0.781113
6	1.017671	-2.847851	-0.740966
6	2.939918	-1.452885	-0.772798
6	2.450114	-2.805791	-1.272838
1	3.074143	-3.625739	-0.915032
1	2.454224	-2.802652	-2.366900
6	-2.234685	-2.486514	0.280971
6	-2.762509	-1.971212	-1.068319
6	-4.269665	-1.763765	-1.119771
6	-4.809414	-0.774147	-0.096555
6	-2.871831	0.691212	0.693724
6	-4.141008	0.599748	-0.140235
1	-3.062482	-2.914527	0.842896
1	-2.294430	-1.030135	-1.476634
1	-4.751303	-2.739553	-0.986555
1	-5.887605	-0.676609	-0.260351
1	-2.513085	1.730655	0.716772
1	-1.466673	-3.246435	0.133255
1	-2.432662	-2.682931	-1.833447

1	-4.536515	-1.425453	-2.128425
1	-4.700677	-1.189644	0.916837
1	-3.099855	0.433769	1.739131
1	-3.940946	0.877726	-1.187433
1	-4.859589	1.350384	0.218879
6	-0.584852	-0.699796	2.055497
1	-0.855184	0.221114	2.568449
1	0.474062	-0.960391	2.072537
6	-1.533828	-1.766066	2.057866
1	-2.501937	-1.565934	2.509388
1	-1.171607	-2.774048	2.238092
6	0.303283	3.802599	0.572212
6	0.422078	3.804411	-0.934706
1	1.068994	4.402913	1.065427
1	-0.687164	4.127285	0.908323
1	1.466754	3.812212	-1.268442
1	-0.116201	4.620633	-1.415726
8	-0.199560	2.563971	-1.353996
8	0.501534	2.425620	0.970283
8	3.835712	-0.737113	-1.556591
8	3.406762	-1.670949	0.547349
6	5.066030	-1.420283	-1.792197
1	5.725055	-0.710689	-2.291830
1	5.527540	-1.750088	-0.855395
1	4.916203	-2.288677	-2.444996
6	3.823535	-0.513139	1.261927
1	4.487244	0.119889	0.661647
1	2.972826	0.086385	1.613440
1	4.374319	-0.874607	2.131042
1	0.971870	-3.304020	0.257033
1	0.333551	-3.401758	-1.390586

L46 – Hexene (PNCN_S_PCp_X-CF3_TS1)
Electronic Energy: -1760.73127807
Enthalpy: -1760.300468
Free Energy: -1760.384546

Cr	-1.441225	-0.651816	-0.412172
P	-0.239095	1.350836	0.289200
N	1.399508	0.743758	0.279588
C	1.608842	-0.514542	-0.153798
N	0.613746	-1.352487	-0.340239
H	2.211835	1.336375	0.401994
C	-0.503586	1.984289	1.997875
C	-0.063169	3.039388	-0.444691
C	1.158029	-2.571565	-0.951711
C	2.959448	-1.041896	-0.515450
C	2.584343	-2.212869	-1.417692
H	3.269371	-3.059240	-1.359197
H	2.548959	-1.888904	-2.460318
H	-2.766903	-1.608421	-0.508425
H	-2.164805	0.672840	-2.537561
H	-2.996921	1.485432	-1.128943
C	-3.426694	-0.639173	-1.316353
C	-2.647062	0.548832	-1.565875
H	-1.583508	1.958029	2.189448
C	-4.642546	-0.525710	-0.403203
H	-4.556972	0.412898	0.163314
H	-5.539121	-0.424228	-1.025679
C	-4.804854	-1.675648	0.586418
H	-4.949059	-2.621299	0.045077
H	-5.713999	-1.519374	1.175027
C	-3.595426	-1.799468	1.510790
H	-3.426881	-0.827860	2.003912
H	-3.809020	-2.506673	2.322435
C	-2.334398	-2.232400	0.776490

H	-1.446125	-2.184013	1.419132
H	-2.408469	-3.258784	0.405694
H	-3.553014	-1.322878	-2.161884
H	-0.030246	1.325421	2.730190
H	0.981895	3.165574	-0.749458
H	-0.669083	3.135808	-1.348487
H	3.578875	-0.287483	-1.006231
H	3.486749	-1.364972	0.387974
C	-0.447425	4.025979	0.662759
C	0.007233	3.423345	1.987553
H	-0.008518	5.009573	0.477660
H	-1.535448	4.160684	0.676800
H	1.103473	3.430124	2.048094
H	-0.363271	3.984543	2.849354
C	0.273541	-2.967533	-2.141827
F	0.894056	-3.834006	-2.944795
F	-0.031164	-1.868267	-2.870163
F	-0.894114	-3.511370	-1.756076
C	1.223731	-3.709648	0.078910
F	2.133906	-3.402975	1.025013
F	1.604428	-4.854702	-0.507350
F	0.062028	-3.928708	0.701162

L46 – Octene (PNCN_S_PCp_X-CF3_TS2)
Electronic Energy: -1839.34128345
Enthalpy: -1838.848158
Free Energy: -1838.936077

Cr	-1.378962	-0.656692	0.406109
P	-0.071535	1.346680	0.037715
N	1.528223	0.742080	-0.268078
C	1.725931	-0.590268	-0.363554
N	0.755933	-1.461655	-0.235855
H	2.332336	1.339350	-0.417705
C	0.174965	2.619492	1.352459
C	-0.352458	2.587515	-1.288660
C	1.349957	-2.797341	-0.355493
C	3.093046	-1.154774	-0.587921
C	2.784287	-2.609974	-0.898484
H	3.484456	-3.319967	-0.456864
H	2.786203	-2.781191	-1.976361
C	-2.704999	-2.386109	0.554955
C	-2.820732	-1.983693	-0.925697
C	-4.221176	-1.592404	-1.377958
C	-4.841038	-0.428966	-0.618070
C	-2.943560	0.741863	0.619323
C	-3.949315	0.806840	-0.520994
H	-3.705421	-2.505685	0.965483
H	-2.139092	-1.160153	-1.291900
H	-4.864725	-2.475561	-1.295526
H	-5.788249	-0.174227	-1.104537
H	-2.528799	1.744088	0.808329
H	-2.155280	-3.318391	0.649376
H	-2.438135	-2.818152	-1.520032
H	-4.176561	-1.347033	-2.446407
H	-5.108411	-0.746459	0.400378
H	-3.460426	0.467957	1.549621
H	-3.445186	0.972505	-1.488387
H	-4.590648	1.689105	-0.382844
C	-1.080451	-0.679969	2.433982
H	-1.328397	0.307124	2.820473
H	-0.078791	-1.041911	2.664615
C	-2.136361	-1.639157	2.357991
H	-3.126637	-1.298303	2.644662
H	-1.924672	-2.657898	2.665469
H	0.041678	2.237067	-2.245571

H	-0.459893	2.408599	2.216890
H	-1.438133	2.694652	-1.403142
H	1.212353	2.538845	1.694553
C	-0.114990	3.979072	0.705558
C	0.264934	3.884635	-0.768507
H	0.419047	4.780710	1.221954
H	-1.184607	4.203937	0.789723
H	1.357189	3.848351	-0.876269
H	-0.080248	4.749285	-1.341607
H	3.626426	-0.635867	-1.388620
H	3.685831	-1.033165	0.324933
C	0.553952	-3.677997	-1.328452
F	1.277172	-4.742584	-1.701072
F	0.239418	-2.982458	-2.434667
F	-0.594122	-4.141783	-0.801263
C	1.389344	-3.434481	1.038262
F	2.218965	-2.729166	1.832733
F	1.832846	-4.696656	0.989300
F	0.183080	-3.439126	1.632788

L47 – Hexene (PNCN_S_PCp_X-CH3_TS1)
Electronic Energy: -1165.35517586
Enthalpy: -1164.882581
Free Energy: -1164.958138

Cr	-1.416546	-0.568329	-0.444351
P	-0.184738	1.402266	0.272309
N	1.434693	0.776851	0.265330
C	1.598397	-0.498623	-0.171787
N	0.581706	-1.280138	-0.409576
H	2.262361	1.345308	0.393134
C	-0.470167	2.049904	1.974225
C	-0.021137	3.086413	-0.474348
C	1.086444	-2.589734	-0.935276
C	2.936292	-1.106512	-0.450772
C	2.535206	-2.265361	-1.358087
H	3.195187	-3.131433	-1.273861
H	2.549628	-1.937532	-2.403135
H	-2.721549	-1.546069	-0.617090
H	-2.260231	0.988008	-2.381516
H	-3.025161	1.611155	-0.846248
C	-3.433497	-0.485420	-1.267347
C	-2.684202	0.738855	-1.407278
H	-1.550283	2.003129	2.162262
C	-4.608129	-0.516076	-0.296138
H	-4.498788	0.329174	0.399235
H	-5.532845	-0.331190	-0.855425
C	-4.722812	-1.802462	0.517214
H	-4.882586	-2.658204	-0.154374
H	-5.609205	-1.747959	1.156650
C	-3.479399	-2.049140	1.368779
H	-3.299618	-1.158727	1.993209
H	-3.657208	-2.871335	2.073497
C	-2.234579	-2.343527	0.537433
H	-1.334322	-2.368371	1.163155
H	-2.306322	-3.313284	0.030705
H	-3.591458	-1.060796	-2.185237
H	0.014622	1.409728	2.715400
H	1.028647	3.225629	-0.756347
H	-0.610367	3.167788	-1.390489
H	3.633450	-0.396302	-0.903468
H	3.392174	-1.443952	0.488313
C	-0.442098	4.076325	0.615762
C	0.011072	3.499086	1.952334
H	-0.025903	5.068763	0.424829
H	-1.533681	4.183524	0.615851

H	1.106401	3.528240	2.022030
H	-0.378557	4.063473	2.803719
C	0.216920	-3.015609	-2.104198
C	1.065025	-3.637558	0.171848
H	0.618881	-3.914540	-2.581471
H	1.470363	-4.584117	-0.198034
H	0.049959	-3.831505	0.525801
H	1.669715	-3.327581	1.030364
H	-0.802207	-3.248920	-1.777128
H	0.167060	-2.227908	-2.864702

L47 – Octene (PNCN_S_PCp_X-CH3_TS2)
Electronic Energy: -1243.9620615
Enthalpy: -1243.427183
Free Energy: -1243.505827

Cr	-1.342829	-0.582571	0.330028
P	-0.024635	1.425277	-0.008735
N	1.560890	0.769990	-0.217634
C	1.699883	-0.581033	-0.329531
N	0.696050	-1.405318	-0.261610
H	2.389683	1.336565	-0.346152
C	0.161684	2.689333	1.325007
C	-0.215704	2.678699	-1.342702
C	1.224011	-2.803283	-0.356306
C	3.049161	-1.213163	-0.482275
C	2.668966	-2.631515	-0.877454
H	3.342924	-3.391673	-0.475500
H	2.677891	-2.729615	-1.967907
C	-2.496394	-2.422491	0.446680
C	-2.748458	-1.966211	-0.999252
C	-4.205510	-1.671300	-1.328574
C	-4.851421	-0.594912	-0.468901
C	-2.962786	0.731570	0.621661
C	-4.073505	0.718249	-0.419109
H	-3.443796	-2.712970	0.896531
H	-2.152866	-1.079266	-1.366040
H	-4.769040	-2.607418	-1.240664
H	-5.863206	-0.421536	-0.850103
H	-2.582143	1.758019	0.738932
H	-1.813084	-3.271423	0.471219
H	-2.350100	-2.742937	-1.661677
H	-4.264937	-1.377333	-2.383898
H	-4.982912	-0.965305	0.558844
H	-3.384404	0.470124	1.603365
H	-3.678268	0.946560	-1.423122
H	-4.780080	1.532625	-0.203264
C	-0.983692	-0.643630	2.351722
H	-1.286986	0.317081	2.763971
H	0.046493	-0.939508	2.547447
C	-1.976011	-1.665011	2.268405
H	-2.984761	-1.398050	2.570167
H	-1.698026	-2.678410	2.545357
H	0.243203	2.333848	-2.272423
H	-0.509397	2.472708	2.160240
H	-1.290209	2.791715	-1.532111
H	1.184163	2.607964	1.709299
C	-0.099789	4.052271	0.675232
C	0.369301	3.970085	-0.773748
H	0.397237	4.853415	1.228327
H	-1.174201	4.269948	0.696806
H	1.466140	3.931936	-0.811683
H	0.062524	4.841237	-1.359026
H	3.576779	-1.163907	0.478557
H	3.677995	-0.693591	-1.211093
C	0.401466	-3.628884	-1.330875

H	0.900856	-4.583839	-1.522082
H	-0.593951	-3.861261	-0.944385
H	0.292430	-3.111835	-2.289446
C	1.197010	-3.417286	1.038219
H	0.183588	-3.395449	1.454163
H	1.524956	-4.460911	1.012286
H	1.852797	-2.874757	1.727877

L48 – Hexene (PNCN_S_PCp_X-F_TS1)
Electronic Energy: -1285.19310714
Enthalpy: -1284.793072
Free Energy: -1284.866299

Cr	-1.448575	-0.521312	-0.497755
P	-0.197040	1.435658	0.219045
N	1.443765	0.827743	0.223603
C	1.617305	-0.444976	-0.170662
N	0.590545	-1.214549	-0.455648
H	2.266689	1.392109	0.398462
C	-0.444428	2.156638	1.894383
C	-0.042228	3.082758	-0.606164
C	1.110321	-2.504273	-0.836420
C	2.953183	-1.102601	-0.325909
C	2.585491	-2.332886	-1.150843
H	3.151890	-3.229860	-0.903780
H	2.693780	-2.132979	-2.218730
H	-2.765299	-1.444180	-0.852089
H	-2.505213	1.337788	-2.070620
H	-3.084747	1.687428	-0.376672
C	-3.541890	-0.316334	-1.090948
C	-2.804697	0.924865	-1.106116
H	-1.521801	2.125961	2.098870
C	-4.546535	-0.539838	0.032604
H	-4.285544	0.131371	0.864943
H	-5.537717	-0.223176	-0.313131
C	-4.590688	-1.970957	0.556912
H	-4.913406	-2.652728	-0.242537
H	-5.348002	-2.043164	1.343760
C	-3.233916	-2.423034	1.089111
H	-2.899703	-1.706107	1.859363
H	-3.332293	-3.383228	1.612253
C	-2.171899	-2.539347	0.001710
H	-1.206533	-2.838578	0.412037
H	-2.444807	-3.288817	-0.750288
H	-3.859251	-0.698360	-2.066391
H	0.044729	1.544760	2.656151
H	0.999312	3.197982	-0.926281
H	-0.659109	3.128522	-1.506261
H	3.690205	-0.446193	-0.794004
H	3.338910	-1.369186	0.664713
C	-0.422998	4.125144	0.450194
C	0.048935	3.599409	1.801135
H	0.007062	5.099889	0.206557
H	-1.511665	4.254026	0.467584
H	1.145426	3.622462	1.852039
H	-0.321588	4.201796	2.634631
F	0.938348	-3.385820	0.201704
F	0.382647	-2.998942	-1.870136

L48 – Octene (PNCN_S_PCp_X-F_TS2)
Electronic Energy: -1363.80467056
Enthalpy: -1363.342920
Free Energy: -1363.421107

Cr	-1.357031	-0.524827	0.349178
P	-0.024951	1.506350	0.013955

N	1.554077	0.824742	-0.305287
C	1.678230	-0.514613	-0.388038
N	0.644833	-1.304719	-0.251563
H	2.386104	1.385379	-0.444900
C	0.291821	2.767186	1.326333
C	-0.251054	2.757628	-1.313072
C	1.095179	-2.659298	-0.329793
C	2.989440	-1.206434	-0.602637
C	2.572600	-2.671446	-0.705656
H	3.128125	-3.329693	-0.038272
H	2.674785	-3.053731	-1.721715
C	-2.304902	-2.473505	0.295139
C	-2.597280	-1.918994	-1.107850
C	-4.072855	-1.718230	-1.421300
C	-4.796072	-0.756169	-0.488971
C	-3.034707	0.659615	0.699196
C	-4.130025	0.613545	-0.356793
H	-3.220679	-2.894171	0.705591
H	-2.084683	-0.955007	-1.391401
H	-4.562925	-2.698552	-1.400005
H	-5.823173	-0.643798	-0.851415
H	-2.708608	1.699410	0.859021
H	-1.535772	-3.241637	0.248371
H	-2.122447	-2.598701	-1.822642
H	-4.158504	-1.356676	-2.453699
H	-4.883188	-1.203736	0.512383
H	-3.444755	0.330146	1.665811
H	-3.741291	0.926676	-1.340494
H	-4.903474	1.355350	-0.111050
C	-0.976638	-0.724903	2.351876
H	-1.364752	0.162488	2.848867
H	0.074748	-0.948537	2.528904
C	-1.869469	-1.825240	2.171702
H	-2.897913	-1.682356	2.491160
H	-1.487950	-2.824674	2.357399
H	0.124479	2.389032	-2.270679
H	-0.341201	2.581310	2.197581
H	-1.331527	2.910861	-1.425741
H	1.328966	2.647782	1.657605
H	3.652171	-1.008754	0.246066
H	3.500596	-0.829770	-1.492843
C	0.049018	4.135966	0.679840
C	0.422161	4.026421	-0.794657
H	0.612442	4.917770	1.195260
H	-1.011822	4.398355	0.766006
H	1.511692	3.943604	-0.904491
H	0.113249	4.905407	-1.366626
F	0.856339	-3.272845	0.874519
F	0.326182	-3.343636	-1.230742

L49 – Hexene (PNCN_S_PCp_X-F_Z-F-TS1)
Electronic Energy: -1285.1943811
Enthalpy: -1284.793801
Free Energy: -1284.865173

Cr	-1.456808	-0.508986	-0.394999
P	-0.196687	1.481702	0.283598
N	1.444298	0.877438	0.147889
C	1.602077	-0.398200	-0.241280
N	0.561781	-1.177068	-0.425200
H	2.271241	1.450067	0.266952
C	-0.306661	2.157534	1.992821
C	-0.085994	3.151440	-0.502396
C	1.037292	-2.461604	-0.864097
C	2.922759	-1.046965	-0.514943
C	2.491599	-2.299971	-1.275029

H	3.071715	-3.191642	-1.041091
H	2.529158	-2.132312	-2.353124
H	-2.671765	-1.556689	-0.724167
H	-2.421101	1.160728	-2.195519
H	-3.202473	1.578520	-0.597831
C	-3.471237	-0.491403	-1.222725
C	-2.812706	0.791663	-1.246696
H	-1.367762	2.146033	2.270207
C	-4.623868	-0.700419	-0.246712
H	-4.567246	0.083489	0.522772
H	-5.568152	-0.535502	-0.778685
C	-4.630388	-2.059924	0.446110
H	-4.752855	-2.861013	-0.296454
H	-5.499354	-2.121880	1.108485
C	-3.348570	-2.298629	1.239934
H	-3.203509	-1.456655	1.938234
H	-3.454794	-3.187475	1.875398
C	-2.118501	-2.447777	0.356443
H	-1.198127	-2.522479	0.944515
H	-2.167144	-3.341772	-0.274930
H	-3.605765	-0.979694	-2.192772
H	0.219340	1.511735	2.700190
H	0.922104	3.258832	-0.918345
H	-0.785086	3.233606	-1.337521
H	3.597898	-0.393018	-1.071702
H	3.414265	-1.285525	0.434869
C	-0.347537	4.169850	0.611906
C	0.213410	3.590910	1.905471
H	0.088787	5.140370	0.363042
H	-1.427430	4.324841	0.721598
H	1.311269	3.590044	1.878243
H	-0.080455	4.173733	2.782535
F	0.901521	-3.366537	0.152500
F	0.238079	-2.912758	-1.870224

L49 – Octene (PNCN_S_PCp_X-F_Z-F-TS2)
Electronic Energy: -1562.24318834
Enthalpy: -1561.796272
Free Energy: -1561.877786

Cr	-1.378064	-0.529456	0.331584
P	-0.043698	1.512787	-0.007848
N	1.536847	0.820641	-0.336898
C	1.646305	-0.511361	-0.396754
N	0.642009	-1.330235	-0.268558
H	2.381743	1.366586	-0.470985
C	0.290691	2.752191	1.319169
C	-0.245371	2.778432	-1.322729
C	1.130370	-2.680995	-0.330587
C	2.988685	-1.206178	-0.559954
C	2.610528	-2.664050	-0.697538
H	3.198900	-3.304364	-0.042315
H	2.739130	-2.985974	-1.730918
C	-2.315529	-2.479701	0.283568
C	-2.626208	-1.927081	-1.115818
C	-4.105241	-1.723458	-1.410443
C	-4.814973	-0.759829	-0.469514
C	-3.043630	0.662697	0.694883
C	-4.147520	0.610472	-0.350787
H	-3.221316	-2.915265	0.700548
H	-2.112241	-0.965817	-1.407107
H	-4.596346	-2.702988	-1.382254
H	-5.847110	-0.648379	-0.817157
H	-2.709449	1.701703	0.841902
H	-1.534752	-3.236788	0.233796
H	-2.164014	-2.608933	-1.837379

H	-4.203236	-1.362484	-2.441785
H	-4.887662	-1.205363	0.533869
H	-3.443081	0.341701	1.668368
H	-3.767833	0.919863	-1.338949
H	-4.917359	1.354078	-0.099832
C	-0.983441	-0.728665	2.332732
H	-1.361254	0.165041	2.826287
H	0.066154	-0.961399	2.509450
C	-1.887816	-1.820357	2.162528
H	-2.916028	-1.663776	2.476407
H	-1.519886	-2.823382	2.356154
H	0.123755	2.411584	-2.283439
H	-0.351141	2.568230	2.184307
H	-1.322923	2.952633	-1.433639
H	1.323046	2.608358	1.655364
C	0.077683	4.131667	0.684526
C	0.452577	4.028009	-0.789711
H	0.656962	4.895568	1.208806
H	-0.977578	4.415274	0.771409
H	1.540205	3.924384	-0.898380
H	0.162330	4.917517	-1.354918
F	0.904524	-3.280984	0.874829
F	0.387365	-3.380303	-1.232422
F	3.746080	-0.947727	0.542104
F	3.663262	-0.702887	-1.625180

L50 – Hexene (PNCN_S_PCp_X-H_TS1)
Electronic Energy: -1086.67527258
Enthalpy: -1086.260490
Free Energy: -1086.331938

Cr	-1.438713	-0.460853	-0.434031
P	-0.166653	1.487089	0.247718
N	1.453125	0.849413	0.184512
C	1.583120	-0.439137	-0.224174
N	0.539974	-1.172434	-0.505985
H	2.293889	1.391002	0.334657
C	-0.344192	2.221788	1.929150
C	-0.043203	3.131016	-0.592997
C	1.004834	-2.524518	-0.869140
C	2.897200	-1.140520	-0.359698
C	2.496965	-2.371726	-1.173781
H	3.075555	-3.261056	-0.921541
H	2.643452	-2.174879	-2.239441
H	0.424885	-2.904535	-1.714327
H	-2.703040	-1.449030	-0.738809
H	-2.533379	1.389060	-1.995555
H	-3.172772	1.658944	-0.308331
C	-3.512879	-0.340818	-1.092550
C	-2.839753	0.933551	-1.053374
H	-1.412003	2.199058	2.178183
C	-4.592268	-0.642690	-0.059456
H	-4.441096	0.022886	0.803098
H	-5.565814	-0.372005	-0.483758
C	-4.600175	-2.088187	0.429589
H	-4.785752	-2.768248	-0.413746
H	-5.434191	-2.231400	1.122578
C	-3.286880	-2.463263	1.112085
H	-3.101339	-1.749973	1.931011
H	-3.376546	-3.444318	1.594808
C	-2.090590	-2.468152	0.164018
H	-1.153618	-2.607242	0.714443
H	-2.157112	-3.278874	-0.571462
H	-3.724689	-0.735490	-2.091494
H	0.823706	-3.203906	-0.025847
H	0.173542	1.615750	2.676033

H	0.984514	3.244122	-0.954853
H	-0.695208	3.172279	-1.468005
H	3.665268	-0.518451	-0.827671
H	3.265351	-1.399612	0.641603
C	-0.381947	4.180282	0.471395
C	0.147902	3.663578	1.804398
H	0.032768	5.155510	0.205034
H	-1.469649	4.305571	0.533768
H	1.245649	3.687305	1.808482
H	-0.183454	4.273220	2.648803

L50 – Octene (PNCN_S_PCp_X-H_TS2)
Electronic Energy: -1165.28527978
Enthalpy: -1164.809524
Free Energy: -1164.884845

Cr	-1.330670	-0.509339	0.383526
P	-0.008086	1.497918	0.024300
N	1.555432	0.804444	-0.280243
C	1.656296	-0.551764	-0.365509
N	0.624309	-1.331249	-0.225232
H	2.388174	1.349825	-0.458879
C	0.280169	2.771999	1.333352
C	-0.257481	2.743525	-1.308056
C	1.085560	-2.725773	-0.287617
C	2.963280	-1.254491	-0.569720
C	2.497891	-2.676533	-0.882381
H	3.157038	-3.444511	-0.475947
H	2.452258	-2.824330	-1.964717
H	0.395827	-3.324956	-0.890972
C	-2.269254	-2.470401	0.325391
C	-2.540047	-1.921561	-1.085890
C	-4.012202	-1.720679	-1.418700
C	-4.742207	-0.745316	-0.505007
C	-3.000421	0.708405	0.666877
C	-4.083918	0.630850	-0.400381
H	-3.184780	-2.920121	0.704866
H	-2.016530	-0.961082	-1.363783
H	-4.504681	-2.699557	-1.392862
H	-5.768798	-0.647411	-0.871438
H	-2.680910	1.753872	0.800063
H	-1.483209	-3.225279	0.302083
H	-2.061883	-2.605041	-1.796868
H	-4.085690	-1.370520	-2.455548
H	-4.831246	-1.173304	0.504934
H	-3.426085	0.412984	1.637850
H	-3.686321	0.920645	-1.387654
H	-4.861982	1.375333	-0.181950
C	-1.001494	-0.711688	2.392108
H	-1.381773	0.186102	2.875323
H	0.038549	-0.957691	2.603555
C	-1.920119	-1.791472	2.198864
H	-2.955890	-1.609089	2.473109
H	-1.584692	-2.797311	2.435325
H	0.135717	2.385725	-2.262419
H	-0.339105	2.568454	2.210278
H	1.073621	-3.149454	0.727425
H	-1.340873	2.866960	-1.428988
H	1.323851	2.687225	1.654130
H	3.546769	-1.194166	0.358148
H	3.572830	-0.797662	-1.354677
C	-0.009418	4.131734	0.686355
C	0.375630	4.033385	-0.786194
H	0.522821	4.933504	1.203977
H	-1.078994	4.357854	0.768210
H	1.468059	3.984435	-0.888625

H 0.045689 4.902853 -1.360495

L51 – Hexene (PNCN_S_PCp_X-H_Z-CH3-TS1)
Electronic Energy: -1165.35086060
Enthalpy: -1164.877675
Free Energy: -1164.954197

24	-1.428345	-0.482617	-0.526322
15	-0.117825	1.449584	0.153318
7	1.479685	0.763658	0.186220
6	1.593919	-0.523341	-0.224788
7	0.545782	-1.231080	-0.550480
1	2.329090	1.291374	0.347470
6	0.999749	-2.583041	-0.923729
6	2.916626	-1.254968	-0.291987
6	2.497732	-2.441880	-1.177910
1	3.060087	-3.350935	-0.950611
1	2.676763	-2.193923	-2.229830
1	-2.735267	-1.432460	-0.800003
1	-2.535143	1.387639	-2.061631
1	-3.100239	1.687973	-0.353423
6	-3.525488	-0.308512	-1.109858
6	-2.816182	0.947761	-1.103951
6	-4.557928	-0.582985	-0.024066
1	-4.319496	0.044890	0.847667
1	-5.540247	-0.249687	-0.379257
6	-4.612790	-2.042089	0.419057
1	-4.863784	-2.681104	-0.439647
1	-5.423655	-2.172244	1.142395
6	-3.292444	-2.502503	1.032210
1	-3.054319	-1.840524	1.879874
1	-3.407913	-3.504118	1.466305
6	-2.124302	-2.499152	0.049177
1	-1.180072	-2.685109	0.571335
1	-2.231176	-3.282040	-0.711926
1	-3.800129	-0.697483	-2.095708
6	-0.268283	4.153044	0.281301
6	0.184450	3.666847	1.653796
1	0.187150	5.107166	0.003704
1	-1.353785	4.308948	0.287479
1	1.281137	3.662417	1.707030
1	-0.171549	4.310974	2.462178
6	4.036910	-0.417828	-0.893430
6	3.289283	-1.713532	1.123751
1	0.441912	-2.936425	-1.795122
1	0.781987	-3.279458	-0.103077
1	4.936148	-1.028035	-1.015224
1	3.767750	-0.023016	-1.877935
1	4.314296	0.424770	-0.249494
1	3.425269	-0.863362	1.799731
1	2.525071	-2.367178	1.555633
1	4.229910	-2.270826	1.097412
6	0.092110	3.061566	-0.730290
6	-0.347400	2.241948	1.800078
1	1.140842	3.133250	-1.039803
1	-0.511352	3.093009	-1.640083
1	0.127778	1.648340	2.584664
1	-1.424215	2.249649	2.007862

L51 – Octene (PNCN_S_PCp_X-H_Z-CH3-TS2)
Electronic Energy: -1243.95886448
Enthalpy: -1243.423768
Free Energy: -1243.504686

Cr	-1.335679	-0.498982	0.361526
P	-0.009148	1.523384	0.012012

N	1.546283	0.821933	-0.303015
C	1.647663	-0.531982	-0.385492
N	0.615842	-1.311861	-0.241323
H	2.378304	1.370089	-0.485742
C	0.309235	2.805000	1.305081
C	-0.258815	2.757761	-1.328730
C	1.080280	-2.704847	-0.308789
C	2.980927	-1.233218	-0.552146
C	2.478722	-2.639752	-0.919623
H	3.143999	-3.428555	-0.560065
H	2.413048	-2.732687	-2.009145
C	-2.266644	-2.457662	0.295320
C	-2.568304	-1.898579	-1.104716
C	-4.049524	-1.725789	-1.410849
C	-4.781959	-0.778882	-0.469972
C	-3.035249	0.668277	0.704637
C	-4.139591	0.602804	-0.342025
H	-3.174669	-2.901295	0.699383
H	-2.081366	-0.919152	-1.377442
H	-4.521898	-2.714863	-1.390339
H	-5.814353	-0.686135	-0.823012
H	-2.722044	1.713948	0.851908
H	-1.486773	-3.217575	0.248589
H	-2.086536	-2.560515	-1.832992
H	-4.147221	-1.361169	-2.441006
H	-4.851417	-1.229992	0.531289
H	-3.439280	0.347413	1.677252
H	-3.763455	0.921115	-1.328999
H	-4.925695	1.330069	-0.092738
C	-0.962192	-0.710713	2.366883
H	-1.351812	0.178281	2.859546
H	0.088911	-0.932197	2.551508
C	-1.858395	-1.806107	2.177527
H	-2.890323	-1.655207	2.482112
H	-1.493183	-2.809588	2.377615
H	0.111804	2.379320	-2.284476
H	-0.312690	2.627943	2.186179
H	-1.340856	2.904995	-1.434328
H	1.351215	2.696562	1.624907
C	0.050757	4.163212	0.643243
C	0.412154	4.036928	-0.833142
H	0.612522	4.956379	1.143215
H	-1.011383	4.419055	0.734509
H	1.501205	3.957224	-0.950373
H	0.094496	4.907532	-1.413311
C	3.871030	-0.611129	-1.619366
H	4.225385	0.385001	-1.329972
H	4.761522	-1.228192	-1.768643
H	3.359645	-0.526561	-2.582949
C	3.696441	-1.230316	0.805051
H	4.643385	-1.771774	0.726936
H	3.922874	-0.212658	1.139664
H	3.098153	-1.713836	1.584343
H	1.084128	-3.131589	0.705294
H	0.386299	-3.306573	-0.904067

L52 – Hexene (PNCN_S_PCp_X-H_Z-F-TS1)
Electronic Energy: -1285.11918884
Enthalpy: -1284.719080
Free Energy: -1284.794936

24	-1.434096	-0.495034	-0.464443
15	-0.127119	1.441204	0.225652
7	1.482393	0.761062	0.185294
6	1.567609	-0.524279	-0.210721
7	0.538407	-1.257693	-0.518955

1	2.348876	1.267120	0.326158
6	1.010904	-2.612670	-0.879789
6	2.878209	-1.278255	-0.286716
6	2.514515	-2.477562	-1.127547
1	3.095427	-3.357257	-0.850790
1	2.716330	-2.238781	-2.174574
1	-2.711890	-1.454446	-0.796332
1	-2.481040	1.397366	-2.010052
1	-3.133105	1.650489	-0.324768
6	-3.498140	-0.329798	-1.145831
6	-2.805150	0.932084	-1.078752
6	-4.596668	-0.632227	-0.133478
1	-4.448434	0.015725	0.742707
1	-5.558766	-0.338406	-0.568130
6	-4.634892	-2.086145	0.328399
1	-4.818393	-2.747655	-0.529922
1	-5.481313	-2.228553	1.006114
6	-3.338540	-2.493936	1.024113
1	-3.155705	-1.800939	1.860498
1	-3.449214	-3.483376	1.484569
6	-2.126704	-2.498283	0.096143
1	-1.201466	-2.657149	0.661294
1	-2.190239	-3.295166	-0.654597
1	-3.699696	-0.706987	-2.153685
6	-0.256275	4.140380	0.423446
6	0.251080	3.617022	1.762421
1	0.194911	5.096950	0.149249
1	-1.338797	4.305980	0.480863
1	1.348717	3.602696	1.771593
1	-0.062924	4.244028	2.600611
9	3.873790	-0.501947	-0.781082
9	3.229591	-1.624640	0.986010
1	0.461462	-2.972745	-1.752324
1	0.795204	-3.298810	-0.052708
6	0.047257	3.070635	-0.631905
6	-0.291002	2.194194	1.898725
1	1.077228	3.146247	-0.996802
1	-0.604787	3.123378	-1.506281
1	0.201601	1.577567	2.653882
1	-1.360815	2.209020	2.139537

L52 – Octene (PNCN_S_PCp_X-H_Z-F-TS2)
Electronic Energy: -1363.77961052
Enthalpy: -1363.318069
Free Energy: -1363.397053

Cr	-1.360489	-0.503492	0.364612
P	-0.024532	1.525454	0.007504
N	1.519100	0.811516	-0.365582
C	1.610927	-0.535653	-0.392173
N	0.619170	-1.347442	-0.199232
H	2.360290	1.340018	-0.568441
C	0.338935	2.768569	1.325138
C	-0.270320	2.791010	-1.301415
C	1.122976	-2.731564	-0.223628
C	2.940160	-1.238235	-0.566860
C	2.534834	-2.669695	-0.812931
H	3.238925	-3.371371	-0.365776
H	2.512259	-2.838098	-1.891870
C	-2.284304	-2.464209	0.290921
C	-2.569248	-1.907430	-1.113589
C	-4.046060	-1.734721	-1.439919
C	-4.789842	-0.783896	-0.512160
C	-3.058059	0.664409	0.681149
C	-4.146707	0.597016	-0.380818
H	-3.194428	-2.916006	0.680534

H	-2.078344	-0.928010	-1.380199
H	-4.519058	-2.723422	-1.422273
H	-5.816988	-0.690394	-0.879476
H	-2.740024	1.708463	0.829027
H	-1.498386	-3.218949	0.255170
H	-2.078133	-2.569930	-1.834977
H	-4.129263	-1.373753	-2.472504
H	-4.873621	-1.231463	0.489568
H	-3.474473	0.346820	1.649218
H	-3.757407	0.912795	-1.363261
H	-4.933563	1.326786	-0.142228
C	-1.018516	-0.710701	2.373751
H	-1.415750	0.179690	2.857668
H	0.028891	-0.931077	2.577024
C	-1.912236	-1.807127	2.175211
H	-2.948875	-1.654800	2.462781
H	-1.550226	-2.809364	2.387021
H	0.077753	2.424984	-2.270308
H	-0.275644	2.582097	2.209461
H	-1.350562	2.962805	-1.385849
H	1.382093	2.630947	1.628768
C	0.099612	4.146023	0.696548
C	0.436584	4.043704	-0.787115
H	0.687185	4.914690	1.204717
H	-0.955005	4.422836	0.810538
H	1.521557	3.943558	-0.922797
H	0.129005	4.932560	-1.344319
F	3.655721	-1.081236	0.590040
F	3.683351	-0.674372	-1.556544
H	1.121096	-3.126442	0.800339
H	0.453514	-3.361583	-0.815753

L53 – Hexene (PNCN_S_PMe_X-H_TS1)
Electronic Energy: -1009.31442851
Enthalpy: -1008.938259
Free Energy: -1009.006684

Cr	-1.449351	-0.502428	-0.432128
P	-0.137969	1.451751	0.222071
N	1.468648	0.803312	0.127204
C	1.585523	-0.487660	-0.269378
N	0.535151	-1.224804	-0.513430
H	2.312940	1.347043	0.252774
C	-0.249903	2.126306	1.905056
C	-0.050372	2.940517	-0.814054
C	0.993097	-2.578188	-0.877816
C	2.895201	-1.191480	-0.427791
C	2.475077	-2.425523	-1.225104
H	3.060731	-3.314105	-0.985598
H	2.590467	-2.231381	-2.295402
H	0.389500	-2.968068	-1.701775
H	-2.730934	-1.472254	-0.755562
H	-2.579995	1.384786	-1.934676
H	-3.157148	1.627635	-0.220801
C	-3.544763	-0.353327	-1.027500
C	-2.857696	0.914062	-0.990629
H	0.748775	3.613078	-0.489574
H	-1.210702	2.635340	2.023821
C	-4.570606	-0.668416	0.053790
H	-4.344505	-0.050972	0.935979
H	-5.559875	-0.348867	-0.294793
C	-4.596974	-2.135094	0.473596
H	-4.846460	-2.765075	-0.392111
H	-5.398068	-2.289396	1.203053
C	-3.263300	-2.584251	1.065246
H	-3.023871	-1.931040	1.919822

H	-3.358579	-3.593294	1.486902
C	-2.109268	-2.549968	0.066907
H	-1.157193	-2.751233	0.568073
H	-2.227011	-3.310759	-0.714733
H	-3.813563	-0.724353	-2.021806
H	0.840796	-3.251102	-0.023719
H	-0.197608	1.323374	2.643018
H	0.547089	2.848558	2.102855
H	0.115319	2.666501	-1.858132
H	-0.999381	3.479656	-0.749806
H	3.653722	-0.572638	-0.914277
H	3.281411	-1.445188	0.567799

L53 – Octene (PNCN_S_PMe_X-H_TS2)
Electronic Energy: -1087.92249488
Enthalpy: -1087.485121
Free Energy: -1087.558211

Cr	-1.318708	-0.538554	0.438353
P	0.012277	1.477365	0.104109
N	1.544671	0.785184	-0.307904
C	1.655515	-0.570283	-0.357940
N	0.640675	-1.355176	-0.139699
H	2.366337	1.336679	-0.519833
C	0.377048	2.571222	1.504422
C	-0.350145	2.617762	-1.260972
C	1.108909	-2.746993	-0.191516
C	2.955498	-1.268252	-0.613366
C	2.489862	-2.702977	-0.855662
H	3.176077	-3.450770	-0.455841
H	2.393087	-2.887348	-1.929252
H	0.396298	-3.366359	-0.745464
C	-2.268256	-2.488086	0.322400
C	-2.461898	-1.929288	-1.098264
C	-3.913646	-1.732896	-1.512777
C	-4.701369	-0.770035	-0.634795
C	-3.027245	0.638320	0.676857
C	-4.047535	0.599965	-0.452644
H	-3.211227	-2.911913	0.662010
H	-1.935748	-0.961273	-1.340050
H	-4.402631	-2.714027	-1.523310
H	-5.699652	-0.659182	-1.070819
H	-2.721455	1.677536	0.871846
H	-1.505132	-3.266088	0.328087
H	-1.940968	-2.603109	-1.787775
H	-3.928235	-1.373087	-2.549132
H	-4.860691	-1.217296	0.357940
H	-3.507090	0.299363	1.607937
H	-3.591468	0.918280	-1.405819
H	-4.838006	1.339230	-0.258858
C	-1.066436	-0.755523	2.456926
H	-1.469085	0.140572	2.926762
H	-0.031603	-0.993447	2.702184
C	-1.964869	-1.841338	2.217571
H	-3.010241	-1.676980	2.464589
H	-1.622803	-2.847280	2.444588
H	-0.490071	2.058684	-2.189089
H	-0.546367	3.059050	1.829854
H	1.149617	-3.145634	0.832524
H	-1.279851	3.151747	-1.043586
H	0.766329	1.987154	2.341042
H	3.589124	-1.174159	0.277669
H	3.515243	-0.829234	-1.443883
H	0.443977	3.356163	-1.403563
H	1.100550	3.347166	1.238742

L54 – Hexene (PNCN_S_PPh_X-H_TS1)
Electronic Energy: -1392.75513269
Enthalpy: -1392.265411
Free Energy: -1392.348012

Cr	-1.353665	-0.413254	-0.451931
P	-0.006711	1.519926	0.180604
N	1.582949	0.823038	0.179821
C	1.672080	-0.492325	-0.139693
N	0.613973	-1.199568	-0.430855
H	2.427132	1.320373	0.434303
C	1.041106	-2.579989	-0.721668
C	2.962530	-1.246566	-0.182947
C	2.551444	-2.499679	-0.955662
H	3.079292	-3.397480	-0.631223
H	2.757908	-2.362185	-2.020983
H	0.489556	-2.967896	-1.582327
H	-2.658166	-1.343211	-0.772213
H	-2.406423	1.551417	-1.916681
H	-3.047704	1.710582	-0.214819
C	-3.417854	-0.224323	-1.134582
C	-2.728149	1.036116	-1.011708
C	-4.543167	-0.565268	-0.165124
H	-4.395892	0.015907	0.757490
H	-5.491313	-0.219996	-0.593360
C	-4.619532	-2.048382	0.187221
H	-4.765018	-2.638779	-0.728990
H	-5.501278	-2.231635	0.809028
C	-3.365471	-2.527795	0.915907
H	-3.249130	-1.928267	1.831718
H	-3.505067	-3.561012	1.258891
C	-2.087863	-2.432139	0.081657
H	-1.205656	-2.586241	0.713161
H	-2.061359	-3.196733	-0.704607
H	-3.596722	-0.567830	-2.158845
H	0.790177	-3.221096	0.133540
H	3.769100	-0.672005	-0.646212
H	3.280521	-1.469846	0.843279
C	-0.366936	1.990628	1.892038
C	-1.154171	1.102204	2.637191
C	0.121026	3.156800	2.494946
C	-1.447810	1.369687	3.969610
H	-1.535255	0.195978	2.157492
C	-0.175744	3.421897	3.827491
H	0.720195	3.858526	1.919378
C	-0.957536	2.531587	4.562226
H	-2.061157	0.680253	4.541484
H	0.201592	4.326661	4.294215
H	-1.189477	2.747573	5.600786
C	0.209248	3.059335	-0.744375
C	-0.726856	4.090346	-0.577434
C	1.212061	3.189765	-1.712776
C	-0.648468	5.236972	-1.359997
H	-1.511265	4.000336	0.170863
C	1.287761	4.343387	-2.487321
H	1.935170	2.392017	-1.861022
C	0.358638	5.365900	-2.313957
H	-1.374757	6.031902	-1.221347
H	2.073572	4.440934	-3.230316
H	0.417931	6.263146	-2.922305

L54 – Octene (PNCN_S_PPh_X-H_TS2)
Electronic Energy: -1471.36118346
Enthalpy: -1470.810406
Free Energy: -1470.899854

Cr	-1.244218	-0.529217	0.524767
P	0.114055	1.505793	0.199275
N	1.637040	0.797317	-0.229311
C	1.758731	-0.558281	-0.215847
N	0.743733	-1.344464	-0.005421
H	2.466189	1.348671	-0.411774
C	1.226126	-2.732904	0.000897
C	3.070559	-1.251472	-0.420384
C	2.623612	-2.697258	-0.628369
H	3.305477	-3.425386	-0.186953
H	2.556779	-2.917009	-1.697675
H	0.534802	-3.376187	-0.552983
C	-2.226479	-2.414239	0.027666
C	-2.270020	-1.657834	-1.308191
C	-3.667635	-1.346556	-1.824970
C	-4.514277	-0.492775	-0.890440
C	-2.940470	0.659301	0.757435
C	-3.847775	0.812717	-0.455335
H	-3.206656	-2.846398	0.221962
H	-1.703291	-0.687419	-1.355004
H	-4.178025	-2.294444	-2.032506
H	-5.463182	-0.284001	-1.395751
H	-2.614774	1.647789	1.116890
H	-1.484840	-3.211283	-0.008198
H	-1.698308	-2.245157	-2.036018
H	-3.566907	-0.833633	-2.790066
H	-4.778911	-1.072546	0.006797
H	-3.513586	0.217667	1.587352
H	-3.295090	1.242193	-1.307782
H	-4.634274	1.548370	-0.232319
C	-1.208992	-1.044970	2.508318
H	-1.661876	-0.226749	3.064960
H	-0.200347	-1.325250	2.810580
C	-2.083110	-2.064224	2.024475
H	-3.146193	-1.919281	2.196175
H	-1.768502	-3.099600	2.120517
H	1.242294	-3.099693	1.036984
H	3.686868	-1.123799	0.478358
H	3.641360	-0.831346	-1.253331
C	0.488827	2.751689	1.453172
C	0.124131	2.498460	2.780926
C	1.159930	3.939611	1.128983
C	0.429501	3.422539	3.775266
H	-0.404222	1.580104	3.026858
C	1.468411	4.854964	2.128177
H	1.424721	4.151174	0.095141
C	1.102966	4.596704	3.449081
H	0.138986	3.227294	4.802870
H	1.989379	5.773834	1.876849
H	1.340112	5.317720	4.225583
C	-0.394136	2.418687	-1.282107
C	-1.201763	3.557771	-1.165594
C	-0.139051	1.879658	-2.550328
C	-1.731708	4.154569	-2.305980
H	-1.415140	3.978897	-0.185736
C	-0.670153	2.482898	-3.685196
H	0.481747	0.991214	-2.648189
C	-1.468212	3.619139	-3.564172
H	-2.351417	5.040709	-2.208988
H	-0.458653	2.066939	-4.665787
H	-1.883655	4.087305	-4.451278

L55 – Hexene (PNCN_UN_PCF3_X-H_Z-H-TS1)
Electronic Energy: -1619.48241493
Enthalpy: -1619.183295
Free Energy: -1619.261195

Cr	-1.449290	-0.562788	-0.482649
P	-0.139311	1.352354	0.180980
N	1.468060	0.818107	0.151968
C	1.618880	-0.501487	-0.223791
N	0.573708	-1.285096	-0.488696
H	2.277110	1.396972	0.340607
C	-0.343914	2.058380	1.910467
C	-0.023997	2.948993	-0.800893
C	1.110888	-2.517386	-0.839517
C	2.465420	-2.463057	-0.775366
H	-2.755196	-1.485854	-0.843071
H	-2.547778	1.344606	-1.988826
H	-3.078833	1.630535	-0.264843
C	-3.550823	-0.347562	-1.035262
C	-2.828023	0.897989	-1.033729
C	-4.529364	-0.628602	0.097992
H	-4.257497	0.005070	0.955039
H	-5.528213	-0.303171	-0.214854
C	-4.556281	-2.084998	0.551452
H	-4.886257	-2.728714	-0.276027
H	-5.301523	-2.201261	1.343888
C	-3.191880	-2.555519	1.047768
H	-2.856931	-1.883632	1.855983
H	-3.277469	-3.546249	1.512295
C	-2.134681	-2.598489	-0.049507
H	-1.155361	-2.877761	0.350096
H	-2.390735	-3.324651	-0.830463
H	-3.872967	-0.709874	-2.016701
F	-0.226471	1.055150	2.791406
F	-1.559083	2.603374	2.036485
F	0.579299	2.983391	2.199994
F	-0.008284	2.657635	-2.108303
F	1.098856	3.623231	-0.512547
F	-1.077982	3.727911	-0.541537
N	2.773824	-1.168222	-0.377531
H	3.702828	-0.800939	-0.232731
H	3.235297	-3.190501	-0.969304
H	0.476921	-3.347725	-1.108866

L55 – Octene (PNCN_UN_PCF3_X-H_Z-H-TS2)
Electronic Energy: -1698.09077534
Enthalpy: -1697.730373
Free Energy: -1697.812075

Cr	-1.349617	-0.563072	0.398580
P	0.079537	1.386164	0.175929
N	1.588642	0.783782	-0.289087
C	1.692474	-0.592490	-0.383080
N	0.674388	-1.408671	-0.136122
H	2.385694	1.365303	-0.517053
C	0.486271	2.476118	1.652350
C	-0.228218	2.726163	-1.108327
C	1.172301	-2.685971	-0.344345
C	2.478338	-2.624142	-0.714423
C	-2.277446	-2.496845	0.424645
C	-2.492356	-2.052958	-1.030430
C	-3.951049	-1.890544	-1.429962
C	-4.708481	-0.845055	-0.623062
C	-3.004977	0.703907	0.493936
C	-4.043969	0.531488	-0.604265
H	-3.195287	-2.947708	0.795883
H	-1.970892	-1.105814	-1.352824
H	-4.441731	-2.866331	-1.337703
H	-5.719881	-0.769859	-1.034732
H	-2.676378	1.752299	0.531141

H	-1.465269	-3.221017	0.502922
H	-1.975065	-2.776777	-1.670255
H	-4.837364	-1.192286	0.413240
H	-3.464600	0.507363	1.473570
H	-3.608508	0.745475	-1.593547
H	-4.822656	1.295488	-0.470197
C	-1.134871	-0.607350	2.443396
H	-1.503359	0.347945	2.813573
H	-0.117999	-0.869467	2.732091
C	-2.073146	-1.666820	2.277746
H	-3.122062	-1.440101	2.450776
H	-1.782132	-2.660661	2.604574
F	-0.632495	2.999528	2.161955
F	1.320946	3.473329	1.321768
F	-0.984242	3.700925	-0.594068
F	-0.870313	2.188735	-2.155799
F	0.921192	3.257236	-1.549753
F	1.079356	1.725589	2.589580
H	-3.988964	-1.626294	-2.493585
N	2.796110	-1.273741	-0.737754
H	3.699343	-0.882215	-0.960786
H	3.206062	-3.379698	-0.958074
H	0.554565	-3.560753	-0.209206

L56 – Hexene (PNCN_UN_PCF3_X-H_Z-Me-TS1)
Electronic Energy: -1658.78827067
Enthalpy: -1658.459644
Free Energy: -1658.540090

Cr	-1.438712	-0.562666	-0.429195
P	-0.106192	1.335235	0.265249
N	1.492892	0.782693	0.227136
C	1.627103	-0.536537	-0.161516
N	0.573673	-1.310820	-0.422036
H	2.311708	1.351091	0.406547
C	-0.312439	2.007037	2.008808
C	0.033978	2.955371	-0.672848
C	1.106120	-2.539880	-0.786147
C	2.461484	-2.482929	-0.734005
H	-2.741578	-1.471547	-0.819332
H	-2.503329	1.391384	-1.905114
H	-3.068926	1.622732	-0.184323
C	-3.526296	-0.329325	-1.027959
C	-2.803719	0.914604	-0.971155
C	-4.541042	-0.644906	0.062991
H	-4.283582	-0.058395	0.957358
H	-5.524584	-0.286533	-0.262122
C	-4.602839	-2.122003	0.439068
H	-4.891152	-2.717464	-0.438774
H	-5.391324	-2.273329	1.182121
C	-3.271011	-2.629416	0.986067
H	-2.990741	-2.015327	1.856999
H	-3.385986	-3.649486	1.374416
C	-2.141505	-2.601622	-0.037233
H	-1.184158	-2.865174	0.422253
H	-2.318555	-3.309197	-0.856705
H	-3.814218	-0.666915	-2.028722
F	-0.170522	0.990864	2.871052
F	-1.537154	2.526517	2.153231
F	0.594473	2.944663	2.309594
F	0.027369	2.704761	-1.988659
F	1.175670	3.595602	-0.378977
F	-0.998407	3.749581	-0.374736
N	2.788582	-1.191726	-0.328522
H	3.230432	-3.209520	-0.939565
H	0.470012	-3.369774	-1.052189

C	4.125169	-0.655284	-0.146343
H	4.842616	-1.459817	-0.295979
H	4.332541	0.133008	-0.874078
H	4.255140	-0.266923	0.866438

L56 – Octene (PNCN_UN_PCF3_X-H_Z-Me-TS2)
Electronic Energy: -1737.39673648
Enthalpy: -1737.007225
Free Energy: -1737.092151

Cr	-1.341303	-0.572264	0.427602
P	0.096298	1.371354	0.267473
N	1.618522	0.768342	-0.151612
C	1.704158	-0.605504	-0.307164
N	0.667272	-1.418636	-0.132104
H	2.392541	1.353510	-0.442112
C	0.467512	2.471447	1.745913
C	-0.176694	2.696205	-1.038904
C	1.171698	-2.690690	-0.346583
C	2.495732	-2.621208	-0.646089
C	-2.277090	-2.501962	0.370174
C	-2.474194	-2.002347	-1.070443
C	-3.927742	-1.810147	-1.476135
C	-4.687498	-0.795585	-0.632725
C	-2.990795	0.697916	0.564736
C	-4.018808	0.576593	-0.550316
H	-3.202809	-2.958217	0.714195
H	-1.934066	-1.054612	-1.358229
H	-4.426610	-2.785168	-1.430799
H	-5.695490	-0.699895	-1.048563
H	-2.659900	1.742394	0.650921
H	-1.472505	-3.236185	0.428036
H	-1.961232	-2.711608	-1.729820
H	-4.825313	-1.185262	0.387291
H	-3.461360	0.460302	1.530022
H	-3.571480	0.829845	-1.525119
H	-4.796384	1.337266	-0.393131
C	-1.146805	-0.693514	2.470844
H	-1.524847	0.244658	2.873645
H	-0.132361	-0.961797	2.762619
C	-2.079422	-1.749420	2.254008
H	-3.129974	-1.533384	2.430797
H	-1.786824	-2.754481	2.542600
F	-0.659554	3.020688	2.207555
F	1.330574	3.450889	1.436720
F	-0.993235	3.650310	-0.584723
F	-0.732369	2.125961	-2.119310
F	0.980569	3.261970	-1.415870
F	1.011670	1.721266	2.712428
H	-3.953529	-1.500389	-2.527777
N	2.832222	-1.272981	-0.611833
H	3.233589	-3.371992	-0.877675
H	0.545221	-3.566607	-0.271839
C	4.141244	-0.694574	-0.847367
H	4.882540	-1.492059	-0.846230
H	4.178931	-0.184570	-1.813605
H	4.394157	0.007527	-0.049163

L57 – Hexene (PNCN_UN_PMe_X-H_Z-H-TS1)
Electronic Energy: -1024.15083372
Enthalpy: -1023.810257
Free Energy: -1023.877262

Cr	-1.425969	-0.517994	-0.398963
P	-0.113924	1.459857	0.239481
N	1.497612	0.840404	0.188078

C	1.623693	-0.474573	-0.162559
N	0.568889	-1.256823	-0.405858
H	2.329664	1.395826	0.332819
C	-0.264684	2.188021	1.897279
C	-0.047915	2.920244	-0.838326
C	1.088890	-2.504243	-0.730330
C	2.443584	-2.466937	-0.676877
H	-2.695311	-1.486819	-0.758471
H	-2.536945	1.396522	-1.886370
H	-3.161606	1.584159	-0.182042
C	-3.502358	-0.377825	-1.055075
C	-2.832345	0.896323	-0.963257
H	0.126322	2.620961	-1.873967
H	-1.230897	2.693473	1.982623
C	-4.577451	-0.727192	-0.033314
H	-4.410974	-0.117549	0.866865
H	-5.552473	-0.421924	-0.430878
C	-4.597142	-2.199621	0.366785
H	-4.793308	-2.823070	-0.517298
H	-5.429288	-2.377646	1.054818
C	-3.284368	-2.632059	1.015201
H	-3.092798	-1.982660	1.884344
H	-3.381529	-3.646249	1.423787
C	-2.089688	-2.572097	0.067585
H	-1.155256	-2.766442	0.603931
H	-2.170538	-3.321415	-0.730056
H	-3.719101	-0.729188	-2.069176
H	-0.218593	1.410319	2.662168
H	0.522668	2.923564	2.085274
H	-1.004881	3.447159	-0.790443
H	0.739943	3.613404	-0.529630
N	2.770855	-1.165772	-0.310175
H	3.704289	-0.808549	-0.175583
H	3.202516	-3.209322	-0.857263
H	0.442226	-3.332573	-0.974595

L57 – Octene (PNCN_UN_PMe_X-H_Z-H-TS2)
Electronic Energy: -1102.75859141
Enthalpy: -1102.356563
Free Energy: -1102.427529

Cr	-1.306021	-0.554487	0.483442
P	0.047501	1.461523	0.163008
N	1.588741	0.790859	-0.215486
C	1.680919	-0.572778	-0.331808
N	0.664072	-1.399796	-0.094153
H	2.391935	1.351226	-0.466861
C	0.367932	2.577519	1.555579
C	-0.316789	2.585769	-1.216782
C	1.164955	-2.674850	-0.311883
C	2.470565	-2.610169	-0.678824
C	-2.254863	-2.498284	0.372860
C	-2.416891	-1.969463	-1.062891
C	-3.858188	-1.766717	-1.507669
C	-4.654025	-0.779425	-0.664642
C	-3.002141	0.649914	0.652046
C	-3.993498	0.590031	-0.501708
H	-3.199103	-2.934054	0.693607
H	-1.867662	-1.017800	-1.317219
H	-4.356786	-2.743146	-1.507771
H	-5.643705	-0.671178	-1.120459
H	-2.685252	1.689977	0.823606
H	-1.478656	-3.262642	0.418260
H	-1.891323	-2.666207	-1.725717
H	-3.850415	-1.427985	-2.551162
H	-4.834087	-1.203190	0.334830

H	-3.509570	0.345075	1.579827
H	-3.511527	0.878998	-1.451352
H	-4.781378	1.341204	-0.346850
C	-1.125495	-0.728451	2.513585
H	-1.529329	0.185293	2.946757
H	-0.101944	-0.975946	2.793531
C	-2.030687	-1.805611	2.267575
H	-3.083377	-1.620562	2.464695
H	-1.713032	-2.810721	2.529274
H	-0.442192	2.016563	-2.140939
H	-0.568122	3.059316	1.853262
H	-1.253447	3.113476	-1.014011
H	0.745809	2.010048	2.408526
H	0.470960	3.331156	-1.359418
H	1.087663	3.358754	1.295027
N	2.786245	-1.257623	-0.691644
H	3.689839	-0.864657	-0.906696
H	0.546305	-3.550840	-0.187932
H	3.198654	-3.363457	-0.928535

L58 – Hexene (PNCN_UN_PMe_X-H_Z-Me-TS1)
Electronic Energy: -1063.45615740
Enthalpy: -1063.085918
Free Energy: -1063.156845

Cr	-1.420279	-0.533118	-0.346334
P	-0.068388	1.417379	0.297888
N	1.529861	0.769805	0.227803
C	1.627075	-0.548059	-0.126476
N	0.557337	-1.316375	-0.349011
H	2.374669	1.315510	0.331066
C	-0.196122	2.139637	1.960412
C	0.016641	2.882363	-0.772361
C	1.062053	-2.566692	-0.681567
C	2.418129	-2.535220	-0.653864
H	-2.707091	-1.470311	-0.724048
H	-2.474310	1.425655	-1.820310
H	-3.116382	1.598726	-0.121065
C	-3.484683	-0.342174	-1.028786
C	-2.790995	0.916725	-0.909084
H	0.819729	3.558956	-0.465877
H	-1.153603	2.659922	2.054900
C	-4.586839	-0.680412	-0.032477
H	-4.428105	-0.080551	0.875563
H	-5.547703	-0.354411	-0.447629
C	-4.641225	-2.155168	0.355751
H	-4.831112	-2.768416	-0.536830
H	-5.490349	-2.322668	1.025486
C	-3.349825	-2.616478	1.027370
H	-3.164040	-1.976285	1.904470
H	-3.474425	-3.631236	1.426962
C	-2.135466	-2.572744	0.104025
H	-1.214283	-2.785380	0.656424
H	-2.213714	-3.316508	-0.699026
H	-3.688525	-0.677012	-2.051110
H	-0.157229	1.357080	2.720718
H	0.604426	2.861071	2.147100
H	0.178575	2.585517	-1.810731
H	-0.929321	3.427751	-0.715512
N	2.774642	-1.237221	-0.291348
H	3.170070	-3.282669	-0.847537
H	0.406275	-3.392518	-0.910081
C	4.119043	-0.715669	-0.150786
H	4.341781	0.015371	-0.933236
H	4.258787	-0.253959	0.830225
H	4.824774	-1.540052	-0.238854

L58 – Octene (PNCN_UN_PMe_X-H_Z-Me-TS2)
Electronic Energy: -1142.06366500
Enthalpy: -1141.632430
Free Energy: -1141.709219

Cr	-1.304813	-0.561282	0.493225
P	0.049979	1.451454	0.144002
N	1.565198	0.773867	-0.314233
C	1.688257	-0.593549	-0.281568
N	0.677710	-1.418046	-0.009393
H	2.387754	1.327711	-0.511466
C	0.419755	2.526131	1.559457
C	-0.340864	2.614981	-1.192272
C	1.228970	-2.689457	-0.035056
C	2.553997	-2.617223	-0.325467
C	-2.262349	-2.499726	0.304112
C	-2.401632	-1.916553	-1.113322
C	-3.835457	-1.691987	-1.571819
C	-4.643193	-0.735175	-0.705428
C	-3.001548	0.637150	0.679994
C	-3.983596	0.625917	-0.482924
H	-3.214659	-2.939272	0.594685
H	-1.842985	-0.960131	-1.325040
H	-4.336123	-2.666389	-1.616153
H	-5.625918	-0.609021	-1.171751
H	-2.683033	1.668406	0.896627
H	-1.495025	-3.273420	0.319599
H	-1.869828	-2.593196	-1.791542
H	-3.810943	-1.314776	-2.601785
H	-4.838652	-1.195016	0.275099
H	-3.518291	0.297806	1.590825
H	-3.493822	0.951285	-1.416560
H	-4.772486	1.370871	-0.304737
C	-1.149515	-0.811718	2.512698
H	-1.563196	0.080150	2.981019
H	-0.128118	-1.065734	2.794282
C	-2.047484	-1.884601	2.213054
H	-3.101481	-1.713227	2.415760
H	-1.725517	-2.896447	2.443385
H	-0.501283	2.072911	-2.127021
H	-0.502256	3.010720	1.894152
H	-1.261742	3.151343	-0.946112
H	0.809089	1.928813	2.386834
H	0.454040	3.351759	-1.339469
H	1.143548	3.305390	1.303838
N	2.843576	-1.265108	-0.479869
H	0.633470	-3.567787	0.164138
H	3.319953	-3.367035	-0.440937
C	4.128460	-0.679966	-0.802038
H	4.138161	-0.281521	-1.820466
H	4.372597	0.118716	-0.096155
H	4.896256	-1.448166	-0.724193

L59 – Hexene (PNCN_UN_PPh_X-CF3_Z-H-TS1)
Electronic Energy: -1744.59260295
Enthalpy: -1744.129936
Free Energy: -1744.218878

Cr	-1.351116	-0.537119	-0.517647
P	-0.025070	1.420203	0.168044
N	1.551824	0.716832	0.328486
C	1.688138	-0.576299	-0.084383
N	0.667380	-1.307511	-0.536348
H	2.351871	1.195538	0.721827
C	1.239899	-2.487555	-0.989996

C	2.582847	-2.475925	-0.787698
H	-2.709365	-1.447769	-0.612028
H	-2.445692	1.262857	-2.110156
H	-2.977873	1.662663	-0.410313
C	-3.466011	-0.358684	-1.047768
C	-2.730159	0.879965	-1.129337
C	-4.515930	-0.521590	0.045849
H	-4.289871	0.192234	0.852478
H	-5.489390	-0.221843	-0.359217
C	-4.588583	-1.927656	0.633816
H	-4.823053	-2.650528	-0.160492
H	-5.415767	-1.981212	1.348392
C	-3.283199	-2.326862	1.318696
H	-3.068648	-1.596107	2.113951
H	-3.410573	-3.287903	1.833787
C	-2.101249	-2.422460	0.359500
H	-1.154261	-2.548335	0.898470
H	-2.208765	-3.282617	-0.307459
H	-3.740048	-0.815684	-2.004020
C	-0.529445	1.919964	1.834781
C	-1.458808	1.106510	2.494930
C	-0.014063	3.048714	2.485301
C	-1.868546	1.409176	3.788773
H	-1.866106	0.233488	1.979477
C	-0.423483	3.348015	3.780053
H	0.694039	3.696958	1.973861
C	-1.348463	2.531291	4.429848
H	-2.594300	0.776607	4.291318
H	-0.024221	4.223641	4.282710
H	-1.668275	2.775122	5.438448
C	0.284968	2.964204	-0.726774
C	-0.634727	4.016442	-0.606712
C	1.355102	3.084701	-1.621210
C	-0.471309	5.174768	-1.358417
H	-1.470410	3.936253	0.084791
C	1.515329	4.249193	-2.365402
H	2.068985	2.273282	-1.731302
C	0.603199	5.293423	-2.236887
H	-1.184511	5.986710	-1.254827
H	2.353860	4.338675	-3.049394
H	0.730320	6.200200	-2.820233
N	2.852081	-1.256303	-0.196776
H	3.768285	-0.915575	0.054188
H	3.354215	-3.195348	-1.006186
C	0.443396	-3.558257	-1.636214
F	1.197729	-4.255904	-2.499600
F	-0.600203	-3.031626	-2.320776
F	-0.069416	-4.443044	-0.758555

L59 – Octene (PNCN_UN_PPh_X-CF3_Z-H-TS2)
Electronic Energy: -1823.20180308
Enthalpy: -1822.677406
Free Energy: -1822.771787

Cr	-1.280453	-0.608699	0.595175
P	0.066405	1.431223	0.111131
N	1.557625	0.753447	-0.448202
C	1.782413	-0.578162	-0.226302
N	0.841190	-1.449251	0.134123
H	2.360051	1.335192	-0.655174
C	1.507148	-2.663160	0.221435
C	2.822702	-2.525210	-0.089637
C	-2.458557	-2.392021	0.116243
C	-2.258184	-1.729057	-1.255031
C	-3.546028	-1.301938	-1.947531
C	-4.417013	-0.351274	-1.136985

C	-2.912385	0.691913	0.647521
C	-3.688338	0.897670	-0.645157
H	-3.512273	-2.637196	0.234043
H	-1.578508	-0.831154	-1.292622
H	-4.114159	-2.204499	-2.200908
H	-5.272568	-0.067441	-1.758853
H	-2.546874	1.656733	1.033030
H	-1.866709	-3.299621	0.181684
H	-1.680153	-2.427322	-1.871069
H	-3.281731	-0.826331	-2.901231
H	-4.845210	-0.879394	-0.271978
H	-3.588080	0.302225	1.422779
H	-3.030807	1.271950	-1.445142
H	-4.427412	1.698270	-0.493787
C	-1.458203	-1.034285	2.590600
H	-1.848109	-0.148702	3.089935
H	-0.514588	-1.423279	2.973783
C	-2.411794	-1.970427	2.083037
H	-3.457796	-1.691335	2.173467
H	-2.232836	-3.026423	2.255317
C	0.525052	2.623694	1.393794
C	0.312498	2.275470	2.733211
C	1.144342	3.843128	1.082461
C	0.713814	3.135834	3.750399
H	-0.168728	1.329290	2.970787
C	1.546349	4.696558	2.103185
H	1.300853	4.125198	0.043362
C	1.330357	4.343765	3.435100
H	0.542106	2.864421	4.787422
H	2.025935	5.640054	1.860667
H	1.641952	5.015783	4.229110
C	-0.510756	2.408070	-1.298686
C	-1.283897	3.557029	-1.085152
C	-0.351363	1.916718	-2.601590
C	-1.872904	4.211296	-2.163073
H	-1.426598	3.941014	-0.077854
C	-0.939703	2.578118	-3.674242
H	0.238657	1.020390	-2.777726
C	-1.701929	3.724437	-3.456234
H	-2.465506	5.104260	-1.989309
H	-0.803073	2.198075	-4.682256
H	-2.163212	4.236975	-4.294874
N	2.984254	-1.185402	-0.372499
H	3.851070	-0.738351	-0.631803
H	3.634996	-3.231677	-0.131707
C	0.822433	-3.928782	0.558919
F	1.711603	-4.900338	0.806663
F	0.023991	-4.360558	-0.448053
F	0.028029	-3.800221	1.645520

L60 – Hexene (PNCN_UN_PPh_X-H_Z-H-TS1)
Electronic Energy: -1407.59187140
Enthalpy: -1407.136282
Free Energy: -1407.216279

Cr	-1.327833	-0.436305	-0.416688
P	0.046400	1.492439	0.207071
N	1.641840	0.822953	0.196910
C	1.711361	-0.519275	-0.067666
N	0.631748	-1.262207	-0.323360
H	2.447557	1.285307	0.598512
C	1.107334	-2.537867	-0.599900
C	2.459986	-2.557755	-0.497497
H	-2.643556	-1.333035	-0.777836
H	-2.320438	1.564229	-1.875802
H	-2.975905	1.718798	-0.178622

C	-3.378769	-0.197673	-1.123830
C	-2.663956	1.046195	-0.980170
C	-4.516841	-0.527730	-0.166162
H	-4.363629	0.038175	0.765083
H	-5.454537	-0.156178	-0.595511
C	-4.628043	-2.013497	0.164104
H	-4.788147	-2.586096	-0.761037
H	-5.514241	-2.184389	0.783133
C	-3.386455	-2.536558	0.884330
H	-3.255052	-1.957744	1.811444
H	-3.552706	-3.572139	1.208108
C	-2.108027	-2.458333	0.050455
H	-1.228650	-2.671065	0.668439
H	-2.118271	-3.192848	-0.765121
H	-3.556666	-0.524448	-2.153775
C	-0.321320	1.971110	1.915667
C	-1.101860	1.083048	2.667856
C	0.157794	3.145567	2.509582
C	-1.395632	1.358132	3.998896
H	-1.478417	0.171560	2.194168
C	-0.138525	3.418121	3.840633
H	0.749677	3.848297	1.927391
C	-0.912427	2.527337	4.582737
H	-2.004309	0.669283	4.576572
H	0.232060	4.329794	4.299686
H	-1.144960	2.749075	5.619985
C	0.228081	3.033223	-0.724082
C	-0.731828	4.041010	-0.553883
C	1.219810	3.183041	-1.700253
C	-0.690666	5.184359	-1.343786
H	-1.507041	3.935133	0.201863
C	1.258401	4.333595	-2.482413
H	1.960728	2.401309	-1.845269
C	0.303828	5.332446	-2.307956
H	-1.435753	5.961405	-1.203626
H	2.035249	4.447325	-3.232572
H	0.333820	6.226093	-2.923715
N	2.831599	-1.261909	-0.158614
H	3.775437	-0.935697	-0.017013
H	0.434420	-3.345585	-0.842442
H	3.190175	-3.339694	-0.621800

L60 – Octene (PNCN_UN_PPh_X-H_Z-H-TS2)
Electronic Energy: -1486.19837355
Enthalpy: -1485.683281
Free Energy: -1485.770035

Cr	-1.263640	-0.525557	0.636415
P	0.077153	1.500464	0.115584
N	1.544957	0.767363	-0.439578
C	1.733734	-0.559962	-0.139254
N	0.755340	-1.349594	0.295281
H	2.357475	1.322075	-0.677078
C	1.334517	-2.593775	0.487520
C	2.652496	-2.550496	0.160593
C	-2.144153	-2.410266	-0.010545
C	-2.099339	-1.604816	-1.317302
C	-3.455880	-1.295889	-1.934073
C	-4.391244	-0.489590	-1.043148
C	-2.974079	0.658537	0.742269
C	-3.793142	0.821148	-0.530036
H	-3.107744	-2.912012	0.059292
H	-1.541366	-0.627478	-1.284597
H	-3.929732	-2.243700	-2.215882
H	-5.307092	-0.292010	-1.610394
H	-2.670963	1.642589	1.133457

H	-1.347942	-3.155413	0.002050
H	-1.460542	-2.160669	-2.013330
H	-3.287113	-0.746704	-2.869855
H	-4.703348	-1.100206	-0.182144
H	-3.606589	0.212550	1.525249
H	-3.189743	1.282646	-1.328913
H	-4.612144	1.532805	-0.349767
C	-1.429225	-1.110213	2.587340
H	-1.922626	-0.305571	3.129774
H	-0.462659	-1.424784	2.980166
C	-2.262117	-2.098994	1.973746
H	-3.335664	-1.935524	2.026653
H	-1.984945	-3.143364	2.091075
C	0.549461	2.704943	1.379387
C	0.273420	2.401160	2.718407
C	1.231732	3.887953	1.060351
C	0.677619	3.269339	3.727858
H	-0.261769	1.485118	2.962247
C	1.636874	4.748586	2.073625
H	1.433635	4.136494	0.020412
C	1.360116	4.439314	3.405232
H	0.457059	3.033982	4.764448
H	2.165875	5.663971	1.826078
H	1.675090	5.116625	4.193400
C	-0.488353	2.448324	-1.318646
C	-1.210176	3.636292	-1.144056
C	-0.366650	1.897393	-2.602193
C	-1.784035	4.270301	-2.242439
H	-1.322724	4.067575	-0.152184
C	-0.940611	2.537858	-3.694724
H	0.187093	0.972443	-2.746336
C	-1.650472	3.723930	-3.516055
H	-2.335453	5.194623	-2.099970
H	-0.832002	2.111434	-4.687557
H	-2.099461	4.221523	-4.370227
N	2.893528	-1.242211	-0.238755
H	3.781613	-0.869457	-0.538087
H	0.756919	-3.428328	0.857505
H	3.433445	-3.292645	0.168327

L61 – Hexene *(PNCN_UN_PPh_X-H_Z-Me-TS1)*

Electronic Energy:

Enthalpy:

Free Energy

24	-1.328463	-0.454441	-0.421003
15	0.038645	1.492939	0.189744
7	1.632152	0.822299	0.215048
6	1.703212	-0.524601	-0.034981
7	0.629602	-1.271358	-0.304797
1	2.422783	1.279411	0.651400
6	1.118639	-2.544967	-0.559840
6	2.469641	-2.551139	-0.430174
1	-2.647383	-1.359215	-0.758281
1	-2.354326	1.526389	-1.889704
1	-2.985851	1.695473	-0.184846
6	-3.391038	-0.232457	-1.104053
6	-2.680266	1.016231	-0.983345
6	-4.513887	-0.557132	-0.126178
1	-4.345571	0.014290	0.799013
1	-5.458888	-0.189157	-0.542403
6	-4.617590	-2.040819	0.216197
1	-4.790121	-2.620315	-0.702218
1	-5.493996	-2.209039	0.849720
6	-3.363924	-2.555950	0.920853
1	-3.219168	-1.970557	1.841838

1	-3.522235	-3.589772	1.254165
6	-2.098626	-2.480061	0.067008
1	-1.210573	-2.690896	0.672294
1	-2.121155	-3.216582	-0.746440
1	-3.583072	-0.570343	-2.127835
6	-0.356221	1.983387	1.889735
6	-1.123001	1.085714	2.645342
6	0.092072	3.173461	2.476767
6	-1.434716	1.367501	3.970705
1	-1.474197	0.159523	2.181190
6	-0.222543	3.453138	3.802419
1	0.674163	3.882802	1.892863
6	-0.983503	2.553228	4.547058
1	-2.031799	0.669924	4.549915
1	0.124141	4.376963	4.255526
1	-1.229851	2.779961	5.580014
6	0.243163	3.025979	-0.748724
6	-0.711017	4.044240	-0.609350
6	1.260142	3.160069	-1.701342
6	-0.636938	5.182977	-1.403979
1	-1.506262	3.950755	0.126937
6	1.330285	4.304868	-2.489415
1	1.996871	2.370339	-1.822767
6	0.383479	5.315490	-2.343165
1	-1.376919	5.968738	-1.286573
1	2.126104	4.405644	-3.221335
1	0.439058	6.206071	-2.961695
7	2.838509	-1.249726	-0.099437
1	0.457090	-3.359628	-0.810410
1	3.209395	-3.328417	-0.533826
6	4.181039	-0.764822	0.145974
1	4.344678	0.180400	-0.377889
1	4.364513	-0.625274	1.215182
1	4.894621	-1.492745	-0.237002

L61 – Octene (PNCN_UN_PPh_X-H_Z-Me-TS2)
Electronic Energy: -1525.50342514
Enthalpy: -1524.958773
Free Energy: -1525.049070

Cr	-1.253407	-0.533370	0.625493
P	0.089894	1.494675	0.133513
N	1.573734	0.772131	-0.387834
C	1.749504	-0.564395	-0.112090
N	0.753337	-1.368611	0.253479
H	2.396747	1.332504	-0.570893
C	1.331523	-2.614408	0.428872
C	2.661945	-2.549469	0.160962
C	-2.152792	-2.413249	-0.009514
C	-2.106951	-1.611578	-1.318787
C	-3.464070	-1.290638	-1.928000
C	-4.390897	-0.481868	-1.030470
C	-2.957944	0.658484	0.747690
C	-3.785419	0.825800	-0.518606
H	-3.122689	-2.901394	0.068987
H	-1.535071	-0.641949	-1.292834
H	-3.945626	-2.234359	-2.210546
H	-5.309228	-0.279920	-1.592162
H	-2.650251	1.641444	1.138048
H	-1.367384	-3.169311	-0.000498
H	-1.478662	-2.176614	-2.016924
H	-3.296159	-0.739555	-2.862822
H	-4.700391	-1.092721	-0.168647
H	-3.586364	0.213425	1.534554
H	-3.186531	1.287750	-1.320584
H	-4.601374	1.539097	-0.330877

C	-1.401268	-1.115923	2.579819
H	-1.884637	-0.307681	3.125996
H	-0.431879	-1.434840	2.962095
C	-2.245640	-2.100847	1.976631
H	-3.317690	-1.932144	2.041703
H	-1.971746	-3.146311	2.091394
C	0.539731	2.707240	1.398075
C	0.263216	2.403144	2.736795
C	1.213234	3.895201	1.078919
C	0.658422	3.276039	3.745790
H	-0.264836	1.482919	2.980319
C	1.609327	4.760674	2.091723
H	1.415618	4.143506	0.038979
C	1.332300	4.451080	3.423120
H	0.437575	3.040466	4.782275
H	2.131530	5.679865	1.843728
H	1.640247	5.131944	4.210998
C	-0.467882	2.435205	-1.309176
C	-1.204618	3.615410	-1.144324
C	-0.328441	1.882630	-2.590108
C	-1.775790	4.240195	-2.249444
H	-1.331267	4.047668	-0.154586
C	-0.900108	2.513534	-3.689428
H	0.236499	0.963415	-2.726967
C	-1.624947	3.691945	-3.520315
H	-2.338863	5.158584	-2.114355
H	-0.778334	2.085424	-4.680024
H	-2.072408	4.181866	-4.379719
N	2.924370	-1.227816	-0.186064
H	0.746108	-3.466287	0.742729
H	3.448585	-3.286760	0.176820
C	4.214763	-0.659611	-0.518205
H	4.219900	-0.263956	-1.537435
H	4.479580	0.136157	0.183619
H	4.970655	-1.440516	-0.451147

L62 – Hexene (PNCN_UN_PiPr_Z-Me-TS1)
Electronic Energy: -1220.63899980
Enthalpy: -1220.149618
Free Energy: -1220.232991

Cr	-1.387387	-0.445656	-0.435425
P	0.008081	1.505699	0.102953
N	1.604082	0.842436	-0.050040
C	1.650687	-0.519982	-0.208635
N	0.554308	-1.269355	-0.342464
H	2.432938	1.311184	0.290245
C	-0.190256	1.811381	1.925105
C	0.137611	3.099347	-0.832053
C	1.012756	-2.567591	-0.524516
C	2.368777	-2.583124	-0.493456
H	-2.671194	-1.427595	-0.665009
H	-2.411549	1.302412	-2.176215
H	-3.110626	1.667811	-0.529955
C	-3.429542	-0.368014	-1.193531
C	-2.750203	0.903431	-1.219856
C	-4.581664	-0.577880	-0.216602
H	-4.478661	0.150470	0.601513
H	-5.519279	-0.328848	-0.726386
C	-4.646750	-1.983028	0.375553
H	-4.775094	-2.720970	-0.429036
H	-5.534008	-2.069729	1.009386
C	-3.395997	-2.318121	1.185560
H	-3.278632	-1.562772	1.977762
H	-3.530732	-3.272584	1.709262
C	-2.122549	-2.373026	0.344698

H	-1.232254	-2.456163	0.978051
H	-2.125024	-3.237668	-0.330973
H	-3.575167	-0.849669	-2.166117
H	0.146744	0.843249	2.327965
H	0.018851	2.772418	-1.874375
C	-1.668566	1.963570	2.281930
H	-1.791945	1.999283	3.367848
H	-2.103006	2.881368	1.874178
H	-2.264821	1.120417	1.909181
C	0.674430	2.909055	2.530493
H	0.364978	3.903599	2.196316
H	0.586635	2.894530	3.620842
H	1.735917	2.788540	2.292047
C	-1.023447	4.030409	-0.492085
H	-0.937359	4.431170	0.522503
H	-1.020962	4.884192	-1.174612
H	-1.997818	3.543694	-0.583829
C	1.484163	3.805245	-0.710465
H	2.314601	3.172845	-1.034849
H	1.488633	4.688378	-1.355527
H	1.682149	4.151596	0.307570
N	2.773074	-1.263829	-0.294579
H	3.090313	-3.377787	-0.591546
H	0.326801	-3.389140	-0.658514
C	4.132200	-0.771547	-0.200660
H	4.282583	0.065603	-0.887510
H	4.371806	-0.457028	0.819405
H	4.817248	-1.568996	-0.483079

L62 – Octene (PNCN_UN_PiPr_Z-Me-TS2)
Electronic Energy: -1299.30592228
Enthalpy: -1298.753806
Free Energy: -1298.836904

24	-1.371826	-0.473884	0.541212
15	-0.007617	1.552194	0.092947
7	1.461971	0.817922	-0.442403
6	1.596520	-0.542814	-0.334933
7	0.593669	-1.357519	-0.011462
1	2.238339	1.351331	-0.810230
6	0.551710	2.631310	1.492056
6	-0.432125	2.643108	-1.340624
6	1.151682	-2.625759	0.019503
6	2.472804	-2.562665	-0.290956
6	-2.292530	-2.436481	0.308538
6	-2.468013	-1.809391	-1.086685
6	-3.915952	-1.621550	-1.517918
6	-4.751725	-0.750922	-0.589922
6	-3.119955	0.633047	0.804706
6	-4.152016	0.626962	-0.314183
1	-3.235079	-2.892576	0.605668
1	-1.949072	-0.826562	-1.275718
1	-4.375146	-2.612686	-1.612531
1	-5.748682	-0.649262	-1.031621
1	-2.821790	1.665573	1.038147
1	-1.521120	-3.204319	0.276098
1	-1.922335	-2.444537	-1.793347
1	-3.920837	-1.185568	-2.525321
1	-4.905205	-1.267565	0.369569
1	-3.587036	0.249154	1.725190
1	-3.723138	1.026582	-1.249137
1	-4.968995	1.319295	-0.062379
6	-1.156391	-0.800323	2.544907
1	-1.596891	0.042938	3.074361
1	-0.117679	-1.021593	2.788246
6	-2.018437	-1.898169	2.223149

1	-3.068752	-1.781436	2.476695
1	-1.645472	-2.903180	2.401359
1	0.479550	3.214750	-1.570008
1	1.148881	1.923046	2.084564
6	-0.797124	1.783791	-2.545275
1	-0.973456	2.416496	-3.420259
1	-0.013066	1.068072	-2.808637
1	-1.723445	1.224779	-2.360754
6	-1.556776	3.613411	-0.998712
1	-1.283450	4.318757	-0.210081
1	-1.817819	4.201481	-1.883642
1	-2.462674	3.084875	-0.681971
6	1.449359	3.779226	1.050471
1	0.903149	4.521766	0.459621
1	1.852331	4.298282	1.925418
1	2.305788	3.439373	0.458056
6	-0.613456	3.094086	2.360242
1	-1.229741	2.253912	2.693627
1	-0.231577	3.600843	3.251508
1	-1.266787	3.802375	1.842827
7	2.754169	-1.218377	-0.511902
1	3.239967	-3.314700	-0.382077
1	0.563106	-3.495991	0.269296
6	4.037734	-0.639815	-0.847907
1	4.056212	-0.283662	-1.881999
1	4.268675	0.189065	-0.173076
1	4.809549	-1.399019	-0.731816

L63 – Hexene (PNCN_UO_PCF3_X-CF3-TS1)
Electronic Energy: -1976.31725927
Enthalpy: -1976.022695
Free Energy: -1976.106727

Cr	-1.492525	-0.686736	-0.539126
P	-0.216177	1.243675	0.157044
N	1.394781	0.678855	0.249745
C	1.561969	-0.589376	-0.213576
N	0.576923	-1.392308	-0.555122
H	2.211559	1.235706	0.480603
C	-0.543985	1.842544	1.907539
C	0.011366	2.891454	-0.721524
C	1.231319	-2.515611	-1.055412
C	2.563343	-2.337187	-0.967103
H	-2.832458	-1.616763	-0.706702
H	-2.480213	0.938962	-2.346689
H	-3.059069	1.567349	-0.730660
C	-3.584530	-0.505227	-1.127138
C	-2.814284	0.693963	-1.336657
C	-4.578857	-0.530055	0.027456
H	-4.306194	0.268635	0.733188
H	-5.568712	-0.266554	-0.361896
C	-4.634687	-1.855179	0.781629
H	-4.963657	-2.657287	0.106468
H	-5.391570	-1.789577	1.568641
C	-3.282782	-2.224486	1.387298
H	-2.942088	-1.395916	2.030922
H	-3.388215	-3.086691	2.058070
C	-2.227122	-2.532088	0.336065
H	-1.240007	-2.703953	0.781240
H	-2.476962	-3.418221	-0.256266
H	-3.911274	-1.031065	-2.029529
F	-0.490500	0.779171	2.722851
F	-1.769525	2.374117	1.971486
F	0.346526	2.746093	2.323698
F	0.104972	2.674694	-2.037421
F	1.125788	3.511812	-0.314318

F	-1.040821	3.676087	-0.478593
H	3.438248	-2.910988	-1.221665
O	2.776949	-1.087821	-0.413425
C	0.472918	-3.665829	-1.615391
F	1.235418	-4.371363	-2.454629
F	-0.609469	-3.214105	-2.290596
F	0.025231	-4.497360	-0.661593

L63 – Octene (PNCN_UO_PCF3_X-CF3-TS2)
Electronic Energy: -2054.92929324
Enthalpy: -2054.572869
Free Energy: -2054.661071

Cr	-1.398193	-0.690786	0.443430
P	0.024696	1.256575	0.076219
N	1.567289	0.674378	-0.338948
C	1.725738	-0.678845	-0.289842
N	0.777800	-1.549903	-0.038994
H	2.368211	1.255925	-0.562743
C	0.450865	2.480144	1.439572
C	-0.324775	2.439963	-1.342931
C	1.455556	-2.765741	-0.076979
C	2.758927	-2.560306	-0.350176
C	-2.635114	-2.469741	0.424466
C	-2.716403	-1.965194	-1.032946
C	-4.109064	-1.579272	-1.510711
C	-4.776528	-0.466451	-0.715569
C	-2.955543	0.684041	0.642248
C	-3.917187	0.781922	-0.529979
H	-3.642399	-2.703891	0.762749
H	-2.041878	-1.108624	-1.324382
H	-4.735623	-2.478019	-1.494309
H	-5.712712	-0.207765	-1.219984
H	-2.545688	1.671897	0.890541
H	-2.020461	-3.365568	0.468395
H	-2.289205	-2.756354	-1.657481
H	-5.069530	-0.839737	0.276757
H	-3.493204	0.358315	1.543111
H	-3.385557	1.016918	-1.466152
H	-4.579852	1.642259	-0.361753
C	-1.176376	-0.855014	2.454028
H	-1.448188	0.096021	2.910612
H	-0.182779	-1.228540	2.703044
C	-2.221682	-1.819627	2.259065
H	-3.226553	-1.503372	2.524053
H	-2.009365	-2.848029	2.535137
F	0.905599	1.791755	2.493570
F	-0.626524	3.176501	1.804753
F	-1.247155	3.333836	-0.982070
F	-0.790523	1.728189	-2.381014
F	0.779632	3.083477	-1.737375
F	1.408139	3.330500	1.044104
H	-4.032012	-1.280268	-2.563022
H	3.630243	-3.180820	-0.474495
O	2.936016	-1.199442	-0.489609
C	0.764305	-4.054181	0.166161
F	1.630494	-5.069436	0.133753
F	-0.191572	-4.281942	-0.760020
F	0.148210	-4.055763	1.367997

L64 – Hexene (PNCN_UO_PCF3_X-CH3-TS1)
Electronic Energy: -1678.63938108
Enthalpy: -1678.323642
Free Energy: -1678.403683

Cr	-1.490021	-0.629652	-0.566641

P	-0.198059	1.279088	0.139187
N	1.398218	0.699866	0.228445
C	1.544650	-0.581530	-0.224487
N	0.551142	-1.354423	-0.610583
H	2.222990	1.240924	0.466783
C	-0.525716	1.910652	1.877163
C	0.024929	2.905663	-0.775094
C	1.179521	-2.539520	-1.039633
C	2.508275	-2.388074	-0.862455
H	-2.828455	-1.557475	-0.756436
H	-2.577842	1.174564	-2.156662
H	-3.089596	1.608024	-0.456828
C	-3.607154	-0.414529	-1.058129
C	-2.861152	0.812167	-1.166643
C	-4.576946	-0.562793	0.108989
H	-4.307554	0.180764	0.873345
H	-5.580066	-0.291266	-0.238775
C	-4.588080	-1.944424	0.755131
H	-4.928748	-2.697398	0.030690
H	-5.319018	-1.952986	1.568961
C	-3.210787	-2.336141	1.284214
H	-2.853139	-1.548273	1.968494
H	-3.281007	-3.243361	1.897633
C	-2.192968	-2.556015	0.174751
H	-1.195013	-2.767487	0.573569
H	-2.474087	-3.394141	-0.473144
H	-3.949402	-0.852697	-2.000741
F	-0.515361	0.858409	2.708991
F	-1.734800	2.481851	1.922197
F	0.388758	2.791148	2.292701
F	0.150662	2.651038	-2.083139
F	1.123261	3.551387	-0.362649
F	-1.040273	3.687093	-0.582386
H	3.380689	-2.993820	-1.036413
O	2.743665	-1.121640	-0.329690
C	0.425156	-3.682956	-1.594623
H	-0.317931	-3.345667	-2.324211
H	1.100059	-4.377884	-2.096176
H	-0.106603	-4.238692	-0.816738

L64 – Octene (PNCN_UO_PCF3_X-CH3-TS2)
Electronic Energy: -1757.24804947
Enthalpy: -1756.870621
Free Energy: -1756.954714

Cr	-1.358807	-0.663878	0.454996
P	-0.003994	1.308254	0.064440
N	1.517745	0.733182	-0.405909
C	1.674787	-0.627346	-0.373310
N	0.730712	-1.496652	-0.098508
H	2.311579	1.313834	-0.653951
C	0.430665	2.524881	1.429366
C	-0.421536	2.495410	-1.331320
C	1.393815	-2.736622	-0.143659
C	2.688005	-2.512218	-0.454857
C	-2.523505	-2.497591	0.410882
C	-2.644042	-1.954182	-1.031273
C	-4.060446	-1.616472	-1.475825
C	-4.759354	-0.556002	-0.636681
C	-2.959810	0.648150	0.710333
C	-3.956233	0.727485	-0.435846
H	-3.515644	-2.790328	0.749105
H	-2.017197	-1.058714	-1.306327
H	-4.648329	-2.541303	-1.476061
H	-5.717684	-0.329159	-1.114456
H	-2.584183	1.648482	0.963854

H	-1.870712	-3.368169	0.419191
H	-2.192793	-2.704082	-1.689799
H	-5.013244	-0.968033	0.351156
H	-3.465762	0.290481	1.618035
H	-3.460752	1.011660	-1.378109
H	-4.657353	1.548575	-0.231394
C	-1.105098	-0.877628	2.456585
H	-1.410686	0.046748	2.944887
H	-0.094664	-1.216157	2.685975
C	-2.116043	-1.877412	2.245894
H	-3.127944	-1.602952	2.531066
H	-1.868718	-2.903118	2.505824
F	-0.655650	3.194272	1.822499
F	1.362375	3.400325	1.028273
F	-1.368277	3.353231	-0.945521
F	-0.881040	1.778535	-2.369431
F	0.651363	3.182922	-1.739978
F	0.917014	1.834770	2.468083
H	-4.014351	-1.283412	-2.519708
H	3.560349	-3.125364	-0.604265
O	2.872106	-1.142649	-0.603938
C	0.716824	-4.020320	0.134953
H	0.248997	-4.017053	1.125182
H	-0.061344	-4.240620	-0.602937
H	1.435406	-4.841176	0.111436

L65 – Hexene (PNCN_UO_PCF3_X-F-TS1)
Electronic Energy: -1738.53276827
Enthalpy: -1738.253862
Free Energy: -1738.332025

Cr	-1.465229	-0.577610	-0.466586
P	-0.171184	1.359398	0.211136
N	1.443264	0.809169	0.272395
C	1.602032	-0.483118	-0.128821
N	0.606427	-1.278466	-0.475506
H	2.264661	1.370258	0.476608
C	-0.406586	2.138577	1.903382
C	-0.002226	2.901543	-0.850722
C	1.257716	-2.447497	-0.824709
C	2.589254	-2.328208	-0.666591
H	-2.760452	-1.504547	-0.838360
H	-2.540124	1.339344	-1.969269
H	-3.125362	1.591814	-0.257255
C	-3.554412	-0.377909	-1.075127
C	-2.845538	0.874528	-1.030662
C	-4.580274	-0.681702	0.008678
H	-4.355165	-0.056695	0.885030
H	-5.564846	-0.360437	-0.349545
C	-4.614179	-2.144521	0.438780
H	-4.881036	-2.780575	-0.416627
H	-5.404888	-2.283886	1.181465
C	-3.275551	-2.596042	1.014942
H	-3.012813	-1.935648	1.857412
H	-3.368120	-3.598858	1.451072
C	-2.143399	-2.598334	-0.003247
H	-1.182744	-2.820803	0.472007
H	-2.294389	-3.345456	-0.790304
H	-3.824529	-0.735800	-2.073734
F	-0.371950	1.168086	2.824800
F	-1.598265	2.741837	1.949990
F	0.547372	3.029266	2.189832
F	-1.089126	3.664969	-0.722181
F	0.120575	2.522922	-2.130136
F	1.078154	3.617823	-0.519564
H	3.453746	-2.950203	-0.808230

O	2.802029	-1.027314	-0.207411
F	0.562572	-3.475611	-1.253121

L65 – Octene (PNCN_UO_PCF3_X-F-TS2)
Electronic Energy: -1817.14388200
Enthalpy: -1816.804612
Free Energy: -1816.885806

Cr	-1.391092	-0.589634	0.392360
P	0.068641	1.361685	0.155439
N	1.586916	0.750573	-0.305067
C	1.680297	-0.607461	-0.408443
N	0.690660	-1.449194	-0.198631
H	2.407991	1.311178	-0.510223
C	0.496396	2.435452	1.639676
C	-0.213698	2.712326	-1.125466
C	1.281740	-2.670318	-0.443584
C	2.578343	-2.534175	-0.781986
C	-2.362045	-2.503911	0.461219
C	-2.559645	-2.084333	-1.003243
C	-4.010478	-1.891267	-1.417400
C	-4.747549	-0.815727	-0.631304
C	-3.017519	0.699657	0.491021
C	-4.045829	0.542267	-0.617766
H	-3.295903	-2.908861	0.844847
H	-2.013196	-1.157551	-1.344589
H	-4.525984	-2.852800	-1.314591
H	-5.750740	-0.715552	-1.056924
H	-2.665860	1.740295	0.533621
H	-1.573765	-3.250010	0.549559
H	-2.055357	-2.836372	-1.620760
H	-4.900397	-1.147307	0.406676
H	-3.483308	0.504175	1.467378
H	-3.594888	0.738957	-1.603643
H	-4.804092	1.328385	-0.495762
C	-1.138539	-0.617109	2.431650
H	-1.477963	0.347876	2.804777
H	-0.121656	-0.899098	2.703658
C	-2.104293	-1.657028	2.299380
H	-3.143528	-1.403233	2.490811
H	-1.830286	-2.653491	2.631985
F	-0.616942	2.965346	2.152436
F	1.339235	3.423306	1.311325
F	-0.965255	3.685350	-0.602719
F	-0.854572	2.187705	-2.178577
F	0.943023	3.233959	-1.550835
F	1.082922	1.669762	2.567241
H	-4.033095	-1.642528	-2.485102
H	3.393521	-3.183746	-1.042760
O	2.830238	-1.164154	-0.754990
F	0.569557	-3.773104	-0.334126

L66 – Hexene (PNCN_UO_PCF3_X-OMe-TS1)
Electronic Energy: -1753.83169388
Enthalpy: -1753.510344
Free Energy: -1753.592152

Cr	-1.493251	-0.633791	-0.542406
P	-0.183603	1.280046	0.132245
N	1.419612	0.714553	0.198852
C	1.563950	-0.584122	-0.196392
N	0.558398	-1.360153	-0.554214
H	2.243971	1.261736	0.424111
C	-0.459541	1.973263	1.856427
C	0.021037	2.882853	-0.828155
C	1.183048	-2.553948	-0.909279

C	2.522384	-2.442657	-0.726744
H	-2.840810	-1.533027	-0.808628
H	-2.560243	1.207533	-2.120482
H	-3.069009	1.622543	-0.415918
C	-3.603579	-0.387666	-1.045021
C	-2.844713	0.833794	-1.135196
C	-4.555483	-0.554721	0.133660
H	-4.251059	0.148634	0.922879
H	-5.557683	-0.242269	-0.181251
C	-4.590035	-1.962845	0.719011
H	-4.966701	-2.672918	-0.030384
H	-5.302699	-1.988810	1.548589
C	-3.213072	-2.415484	1.196962
H	-2.824698	-1.674345	1.917213
H	-3.295506	-3.351353	1.764667
C	-2.216757	-2.599847	0.061469
H	-1.224796	-2.880584	0.425474
H	-2.531442	-3.378699	-0.641778
H	-3.967412	-0.796627	-1.992832
F	-0.371180	0.963199	2.732480
F	-1.682753	2.507950	1.935936
F	0.444224	2.902000	2.185643
F	0.044372	2.608724	-2.137471
F	1.165604	3.500036	-0.507602
F	-1.003907	3.699772	-0.570288
H	3.388375	-3.065678	-0.853889
O	2.754222	-1.139824	-0.259624
O	0.426292	-3.549114	-1.351953
C	1.167759	-4.729580	-1.682536
H	1.706318	-5.102216	-0.804418
H	0.437727	-5.467297	-2.008247
H	1.874325	-4.522838	-2.493746

L67 – Octene (PNCN_UO_PCF3_X-OMe-TS2)
Electronic Energy: -1832.44210939
Enthalpy: -1832.059223
Free Energy: -1832.145873

Cr	-1.380555	-0.591667	0.460532
P	0.088795	1.352412	0.205354
N	1.615637	0.725818	-0.188295
C	1.698180	-0.637068	-0.283017
N	0.700145	-1.467115	-0.075188
H	2.442027	1.275782	-0.398719
C	0.458436	2.507229	1.643343
C	-0.183999	2.626326	-1.151995
C	1.271799	-2.712072	-0.309449
C	2.579401	-2.570235	-0.643035
C	-2.370354	-2.495618	0.585227
C	-2.523111	-2.146349	-0.900785
C	-3.958361	-1.960569	-1.369109
C	-4.713475	-0.848066	-0.655488
C	-3.002592	0.707525	0.440945
C	-4.003693	0.504837	-0.685282
H	-3.317743	-2.872579	0.964528
H	-1.950874	-1.246810	-1.268310
H	-4.484687	-2.913484	-1.241825
H	-5.703407	-0.763223	-1.114584
H	-2.645952	1.747026	0.437576
H	-1.584355	-3.235839	0.729531
H	-2.009703	-2.932574	-1.465413
H	-4.897700	-1.130946	0.391773
H	-3.497979	0.568409	1.412484
H	-3.525212	0.651023	-1.666957
H	-4.759361	1.300418	-0.620703
C	-1.194976	-0.519996	2.509676

H	-1.543075	0.464349	2.818555
H	-0.185899	-0.787634	2.822225
C	-2.157300	-1.562936	2.396487
H	-3.201599	-1.301696	2.545384
H	-1.893338	-2.545162	2.775825
F	-0.680916	3.043628	2.090785
F	1.294634	3.494379	1.294927
F	-1.010664	3.585436	-0.724025
F	-0.738979	2.013382	-2.207887
F	0.965038	3.186912	-1.548008
F	1.023707	1.800876	2.629161
H	-3.945774	-1.757625	-2.446806
H	3.401478	-3.212986	-0.899709
O	2.844543	-1.195767	-0.620761
O	0.502975	-3.791223	-0.184678
C	1.188753	-5.018512	-0.456330
H	2.024761	-5.154001	0.238302
H	0.460901	-5.814857	-0.315529
H	1.556980	-5.030587	-1.487776

L68 – Hexene (PNCN_UO_PMe_X-CF3-TS1)
Electronic Energy: -1380.99042936
Enthalpy: -1380.654471
Free Energy: -1380.728508

Cr	-1.480361	-0.663905	-0.523243
P	-0.210582	1.302632	0.221121
N	1.400229	0.643796	0.340589
C	1.550273	-0.603004	-0.149329
N	0.561355	-1.386985	-0.536507
H	2.235968	1.171126	0.564018
C	-0.560082	1.899836	1.898476
C	0.023178	2.820069	-0.742253
C	1.209660	-2.514920	-1.032109
C	2.541287	-2.365902	-0.902112
H	-2.803186	-1.622532	-0.696177
H	-2.472245	0.958589	-2.335428
H	-3.071680	1.561684	-0.720063
C	-3.563774	-0.514024	-1.136049
C	-2.803699	0.696752	-1.328735
H	0.779127	3.472357	-0.296132
H	-1.543389	2.379372	1.904370
C	-4.576755	-0.549256	0.002601
H	-4.319920	0.250928	0.713295
H	-5.565111	-0.293806	-0.396963
C	-4.631282	-1.873613	0.758450
H	-4.945397	-2.678999	0.079850
H	-5.399342	-1.813860	1.535672
C	-3.283883	-2.234081	1.380057
H	-2.955556	-1.398572	2.022027
H	-3.394190	-3.092744	2.054807
C	-2.215550	-2.535320	0.337232
H	-1.235942	-2.718164	0.793215
H	-2.464276	-3.421751	-0.255571
H	-3.876745	-1.040989	-2.042565
H	-0.586394	1.062333	2.599425
H	0.181112	2.628561	2.238322
H	0.311563	2.578649	-1.767391
H	-0.922909	3.367294	-0.776964
H	3.410175	-2.953909	-1.143476
O	2.764366	-1.130888	-0.321822
C	0.454991	-3.646787	-1.629153
F	1.227396	-4.336379	-2.476521
F	-0.617679	-3.180475	-2.308613
F	-0.006200	-4.505281	-0.703925

L68 – Octene (PNCN_UO_PMe_X-CF3-TS2)
Electronic Energy: -1459.60135669
Enthalpy: -1459.203758
Free Energy: -1459.283253

Cr	-1.347439	-0.663467	0.438424
P	-0.009401	1.345814	0.016733
N	1.531623	0.700022	-0.443458
C	1.679312	-0.641849	-0.391944
N	0.737883	-1.523047	-0.117572
H	2.353761	1.253897	-0.651491
C	0.367940	2.430535	1.419071
C	-0.415776	2.488855	-1.329524
C	1.421712	-2.736243	-0.165806
C	2.717388	-2.528992	-0.467973
C	-2.569910	-2.469047	0.430752
C	-2.681154	-1.959142	-1.018833
C	-4.094042	-1.606290	-1.464223
C	-4.771484	-0.524718	-0.634193
C	-2.943503	0.656671	0.696739
C	-3.941301	0.744449	-0.449390
H	-3.571043	-2.681696	0.800540
H	-2.047052	-1.070592	-1.305009
H	-4.696625	-2.521453	-1.448972
H	-5.727555	-0.284183	-1.110266
H	-2.545725	1.654943	0.934000
H	-1.974907	-3.377672	0.457851
H	-2.240174	-2.724725	-1.665191
H	-4.050410	-1.287061	-2.512922
H	-5.028183	-0.921024	0.359059
H	-3.459746	0.325747	1.609245
H	-3.436200	0.995218	-1.397662
H	-4.626460	1.584231	-0.265457
C	-1.066193	-0.843384	2.447781
H	-1.358152	0.094949	2.917689
H	-0.053520	-1.184618	2.664059
C	-2.082404	-1.838217	2.275180
H	-3.088525	-1.557453	2.573379
H	-1.833410	-2.865960	2.519649
H	0.371504	3.232377	-1.481569
H	-0.558185	2.892604	1.773071
H	-0.573694	1.940063	-2.260509
H	0.792567	1.845765	2.237797
H	-1.340151	3.018075	-1.081056
H	1.065546	3.226255	1.143351
H	3.585575	-3.150279	-0.607426
O	2.889146	-1.169593	-0.616767
C	0.760459	-4.035354	0.095646
F	1.649804	-5.032990	0.054512
F	-0.204082	-4.295833	-0.812932
F	0.166342	-4.049670	1.309155

L69 – Hexene (PNCN_UO_PMe_X-CH3-TS1)
Electronic Energy: -1083.31075997
Enthalpy: -1082.953607
Free Energy: -1083.022807

Cr	-1.471483	-0.603721	-0.545649
P	-0.173747	1.339450	0.185574
N	1.418615	0.661082	0.290397
C	1.541224	-0.603103	-0.177454
N	0.539074	-1.358511	-0.588460
H	2.263928	1.167743	0.522711
C	-0.499179	1.963415	1.859238
C	0.056975	2.846343	-0.797042
C	1.150216	-2.553261	-1.011927

C	2.478275	-2.432907	-0.813504
H	-2.804307	-1.547873	-0.728199
H	-2.565572	1.197394	-2.139140
H	-3.094550	1.611840	-0.442492
C	-3.584776	-0.411995	-1.061815
C	-2.844473	0.822280	-1.152781
H	0.823327	3.496296	-0.365441
H	-1.466974	2.472900	1.869669
C	-4.581938	-0.570197	0.080304
H	-4.327620	0.163579	0.859660
H	-5.578156	-0.292954	-0.283739
C	-4.609424	-1.958952	0.711035
H	-4.924229	-2.703797	-0.033613
H	-5.366609	-1.980284	1.500903
C	-3.248425	-2.354005	1.278956
H	-2.919333	-1.572399	1.984491
H	-3.337298	-3.269646	1.877593
C	-2.190234	-2.547507	0.200392
H	-1.204633	-2.751393	0.632328
H	-2.439598	-3.389384	-0.456088
H	-3.908334	-0.850498	-2.011002
H	-0.541089	1.134652	2.569636
H	0.266479	2.673682	2.183813
H	0.335636	2.592134	-1.821828
H	-0.884534	3.401551	-0.828333
H	3.338548	-3.057881	-0.979375
O	2.733775	-1.175829	-0.268409
C	0.384221	-3.679914	-1.586201
H	-0.165642	-4.234493	-0.820249
H	-0.346108	-3.324819	-2.320490
H	1.053611	-4.381448	-2.086486

L69 – Octene (PNCN_UO_PMe_X-CH3-TS2)
Electronic Energy: -1161.91860071
Enthalpy: -1161.499840
Free Energy: -1161.573984

Cr	-1.329565	-0.637187	0.440767
P	-0.014854	1.388525	0.059467
N	1.509830	0.745659	-0.431253
C	1.658455	-0.603110	-0.384789
N	0.718210	-1.480560	-0.097856
H	2.332072	1.298728	-0.638893
C	0.367525	2.456850	1.474196
C	-0.451089	2.549757	-1.262295
C	1.382598	-2.718710	-0.147469
C	2.673228	-2.496322	-0.470284
C	-2.490849	-2.490999	0.382220
C	-2.596975	-1.959498	-1.060637
C	-4.015709	-1.649354	-1.519898
C	-4.743336	-0.608144	-0.680142
C	-2.975268	0.627021	0.681541
C	-3.969195	0.692339	-0.469747
H	-3.487895	-2.760635	0.725703
H	-1.989505	-1.046373	-1.321601
H	-4.585427	-2.585682	-1.529639
H	-5.705161	-0.401970	-1.160954
H	-2.612698	1.636331	0.927686
H	-1.854491	-3.372771	0.404504
H	-2.121750	-2.696811	-1.716798
H	-3.969564	-1.309180	-2.561826
H	-4.990825	-1.029720	0.305284
H	-3.491642	0.277695	1.587772
H	-3.469686	0.979458	-1.410561
H	-4.691951	1.498315	-0.278568
C	-1.090480	-0.843739	2.454021

H	-1.423563	0.077581	2.929937
H	-0.071647	-1.153670	2.686944
C	-2.070941	-1.867197	2.241239
H	-3.091988	-1.621552	2.519370
H	-1.799962	-2.890402	2.486603
H	-0.613492	2.013482	-2.199838
H	-0.555964	2.918117	1.836325
H	-1.378899	3.063441	-0.994587
H	0.793857	1.862385	2.285012
H	0.325697	3.304609	-1.412781
H	1.066523	3.253671	1.205000
H	3.542951	-3.111981	-0.624265
O	2.856786	-1.127507	-0.625731
C	0.712675	-4.005204	0.138412
H	0.240222	-3.998342	1.126469
H	-0.061706	-4.237379	-0.600059
H	1.436811	-4.821669	0.123296

L70 – Hexene (PNCN_UO_PMe_X-F-TS1)
Electronic Energy: -1143.20583291
Enthalpy: -1142.885503
Free Energy: -1142.954049

Cr	-1.467484	-0.578836	-0.522580
P	-0.162300	1.373636	0.204934
N	1.451665	0.723117	0.245791
C	1.577224	-0.540032	-0.210006
N	0.560828	-1.302975	-0.582873
H	2.295472	1.240703	0.460515
C	-0.413809	2.009410	1.886037
C	0.009714	2.874755	-0.797479
C	1.180113	-2.469327	-0.986554
C	2.514909	-2.391152	-0.838700
H	-2.775357	-1.523625	-0.834715
H	-2.560808	1.283929	-2.057278
H	-3.104266	1.614395	-0.346230
C	-3.571874	-0.381796	-1.064264
C	-2.841852	0.861350	-1.091187
H	0.781430	3.539974	-0.400406
H	-1.385963	2.508142	1.936663
C	-4.554316	-0.615746	0.076823
H	-4.296862	0.071071	0.896921
H	-5.557310	-0.326028	-0.257831
C	-4.562073	-2.040614	0.621342
H	-4.892700	-2.739919	-0.159321
H	-5.298772	-2.113428	1.427201
C	-3.186697	-2.464779	1.128175
H	-2.838093	-1.725669	1.870661
H	-3.257728	-3.413454	1.675670
C	-2.156815	-2.594626	0.011491
H	-1.171405	-2.867801	0.399303
H	-2.439396	-3.367675	-0.712065
H	-3.898494	-0.770584	-2.033803
H	-0.412694	1.189943	2.607919
H	0.357834	2.733021	2.163065
H	0.252000	2.617406	-1.830682
H	-0.941118	3.414709	-0.796049
H	3.360596	-3.028262	-1.019094
O	2.766572	-1.116538	-0.324282
F	0.453589	-3.462183	-1.452661

L70 – Octene (PNCN_UO_PMe_X-F-TS2)
Electronic Energy: -1221.81577619
Enthalpy: -1221.434269
Free Energy: -1221.507929

Cr	-1.343918	-0.582271	0.440935
P	0.037598	1.437559	0.132296
N	1.592192	0.760438	-0.229416
C	1.681200	-0.585029	-0.335413
N	0.688408	-1.436761	-0.148293
H	2.429533	1.299078	-0.416982
C	0.357103	2.530200	1.541111
C	-0.286079	2.573293	-1.244980
C	1.288576	-2.654757	-0.380205
C	2.591440	-2.519059	-0.688860
C	-2.344965	-2.502812	0.393367
C	-2.510717	-1.996288	-1.050547
C	-3.951603	-1.773321	-1.487966
C	-4.716962	-0.753025	-0.655720
C	-3.013003	0.639237	0.636898
C	-4.015929	0.597437	-0.506554
H	-3.302149	-2.882030	0.745262
H	-1.957683	-1.052845	-1.330214
H	-4.470394	-2.738519	-1.465806
H	-5.702309	-0.618250	-1.113324
H	-2.671985	1.671606	0.806605
H	-1.601488	-3.295590	0.434241
H	-1.999902	-2.713680	-1.702861
H	-3.944801	-1.454103	-2.537494
H	-4.911228	-1.159387	0.347971
H	-3.508394	0.335238	1.570650
H	-3.537035	0.872690	-1.461566
H	-4.780118	1.370506	-0.343080
C	-1.095927	-0.729564	2.465203
H	-1.470848	0.192677	2.906583
H	-0.067891	-0.990330	2.716807
C	-2.026193	-1.796183	2.267625
H	-3.066066	-1.590633	2.506425
H	-1.714342	-2.802961	2.528760
H	-0.388888	2.014546	-2.177998
H	-0.580211	3.006456	1.843626
H	-1.228430	3.096977	-1.058039
H	0.733950	1.950929	2.386508
H	0.504482	3.320450	-1.357550
H	1.075727	3.315905	1.292242
H	3.411104	-3.169949	-0.930884
O	2.842290	-1.147927	-0.657504
F	0.577830	-3.762977	-0.288704

L71 – Hexene (PNCN_UO_PMe_X-H-TS1)
Electronic Energy: -1043.9923684
Enthalpy: -1043.664461
Free Energy: -1043.728592

Cr	-1.464381	-0.521721	-0.460864
P	-0.139611	1.440925	0.200270
N	1.473904	0.800102	0.170824
C	1.571261	-0.499317	-0.186559
N	0.543748	-1.280211	-0.467182
H	2.323826	1.320860	0.346877
C	-0.298022	2.138367	1.868095
C	-0.028548	2.909847	-0.857518
C	1.125948	-2.510805	-0.776760
C	2.461283	-2.403925	-0.665559
H	-2.756519	-1.462850	-0.820275
H	-2.566503	1.396020	-1.948752
H	-3.123060	1.636224	-0.226390
C	-3.557607	-0.329586	-1.046707
C	-2.846556	0.923819	-1.006242
H	0.170802	2.618062	-1.890717
H	-1.262094	2.647657	1.953153

C	-4.567752	-0.643855	0.048977
H	-4.315553	-0.043531	0.935930
H	-5.557838	-0.303083	-0.276539
C	-4.610052	-2.116816	0.445471
H	-4.892565	-2.727372	-0.424045
H	-5.395467	-2.268727	1.192089
C	-3.270503	-2.601572	0.994742
H	-2.993927	-1.966334	1.852008
H	-3.374395	-3.614916	1.403548
C	-2.147033	-2.575050	-0.036502
H	-1.186463	-2.826438	0.423309
H	-2.322916	-3.300088	-0.841367
H	-3.846988	-0.683797	-2.041540
H	-0.261147	1.345956	2.617998
H	0.493886	2.864499	2.072378
H	-0.981899	3.444361	-0.830410
H	0.757871	3.589299	-0.517083
H	3.305320	-3.057362	-0.799464
H	0.528698	-3.366528	-1.051499
O	2.754335	-1.098230	-0.280223

L71 – Octene (PNCN_UO_PMe_X-H-TS2)
Electronic Energy: -1122.59966738
Enthalpy: -1122.210954
Free Energy: -1122.282494

Cr	-1.337629	-0.555236	0.456849
P	0.038845	1.457888	0.127271
N	1.570243	0.761757	-0.280540
C	1.641431	-0.590635	-0.344959
N	0.650939	-1.426442	-0.108083
H	2.410440	1.287174	-0.488038
C	0.405610	2.550715	1.525076
C	-0.317546	2.591146	-1.243713
C	1.220315	-2.683906	-0.304951
C	2.512844	-2.537466	-0.648890
C	-2.279340	-2.501251	0.344146
C	-2.467096	-1.958389	-1.083269
C	-3.915754	-1.751037	-1.501212
C	-4.694885	-0.769712	-0.636032
C	-3.019701	0.652063	0.658210
C	-4.030849	0.598521	-0.477637
H	-3.215079	-2.947742	0.674536
H	-1.922843	-1.003583	-1.337181
H	-4.414727	-2.727130	-1.499823
H	-5.693280	-0.658348	-1.071198
H	-2.690836	1.688970	0.825771
H	-1.496583	-3.259812	0.367562
H	-1.952937	-2.648651	-1.761615
H	-3.925984	-1.404362	-2.541910
H	-4.854837	-1.200550	0.363843
H	-3.509216	0.346257	1.595115
H	-3.565939	0.894748	-1.433308
H	-4.814609	1.349107	-0.301958
C	-1.119036	-0.750806	2.479506
H	-1.514994	0.157532	2.930924
H	-0.090848	-1.001045	2.739730
C	-2.028629	-1.826376	2.238735
H	-3.077753	-1.643251	2.455837
H	-1.706678	-2.833399	2.487504
H	-0.453403	2.028215	-2.170048
H	-0.516003	3.046507	1.843613
H	-1.248796	3.124648	-1.031348
H	0.786853	1.966836	2.365397
H	0.476323	3.329685	-1.385663
H	1.135508	3.320242	1.258948

H	0.653332	-3.593663	-0.179454
H	3.331607	-3.192917	-0.889511
O	2.790703	-1.176947	-0.677320

L72 – Hexene (PNCN_UO_PMe_X-OMe-TS1)
Electronic Energy: -1158.50301957
Enthalpy: -1158.140308
Free Energy: -1158.211965

Cr	-1.473065	-0.601459	-0.535144
P	-0.168884	1.348804	0.184280
N	1.432696	0.684802	0.272564
C	1.558939	-0.584778	-0.174504
N	0.546628	-1.335874	-0.576685
H	2.275746	1.194550	0.506420
C	-0.459835	2.006109	1.851668
C	0.036015	2.838678	-0.830210
C	1.154454	-2.526068	-0.963131
C	2.492430	-2.447551	-0.762439
H	-2.799969	-1.537467	-0.791180
H	-2.569427	1.233084	-2.098296
H	-3.093345	1.612066	-0.391969
C	-3.583396	-0.399093	-1.052317
C	-2.842848	0.837398	-1.118579
H	0.805932	3.501292	-0.425144
H	-1.429137	2.512298	1.872827
C	-4.559097	-0.591402	0.102742
H	-4.286160	0.113842	0.902104
H	-5.561965	-0.299066	-0.230272
C	-4.576838	-2.001636	0.684392
H	-4.918937	-2.717183	-0.076608
H	-5.309986	-2.046802	1.495711
C	-3.202130	-2.426501	1.194473
H	-2.846056	-1.673696	1.919314
H	-3.281175	-3.361731	1.764062
C	-2.177129	-2.589226	0.079154
H	-1.188871	-2.851754	0.466457
H	-2.460722	-3.381549	-0.622512
H	-3.924534	-0.808370	-2.008394
H	-0.481772	1.193334	2.580942
H	0.310078	2.726607	2.141720
H	0.297738	2.567040	-1.855042
H	-0.909426	3.387467	-0.855252
H	3.346576	-3.083458	-0.903979
O	2.743820	-1.166908	-0.244075
O	0.384380	-3.493170	-1.451523
C	1.110267	-4.668460	-1.820973
H	1.624283	-5.093950	-0.951919
H	0.375849	-5.377558	-2.197715
H	1.839574	-4.439052	-2.606052

L72 – Octene (PNCN_UO_PMe_X-OMe-TS2)
Electronic Energy: -1237.1137397
Enthalpy: -1236.688786
Free Energy: -1236.765125

Cr	-1.453892	-0.696871	0.437730
P	-0.069263	1.326909	0.138667
N	1.469679	0.651624	-0.265335
C	1.569936	-0.698975	-0.324588
N	0.582823	-1.549893	-0.118348
H	2.312743	1.189158	-0.426444
C	0.269033	2.375605	1.577866
C	-0.397164	2.513601	-1.193019
C	1.188992	-2.788009	-0.282632
C	2.501457	-2.633572	-0.584826

C	-2.494019	-2.590444	0.202113
C	-2.574073	-1.971421	-1.204225
C	-3.984424	-1.675238	-1.695611
C	-4.783755	-0.722970	-0.816271
C	-3.124611	0.521739	0.664025
C	-4.080087	0.600175	-0.516844
H	-3.479637	-2.957405	0.481477
H	-1.970473	-1.034809	-1.383384
H	-4.518252	-2.627828	-1.791956
H	-5.744705	-0.538934	-1.308032
H	-2.776484	1.528080	0.943541
H	-1.775904	-3.406282	0.206398
H	-2.052024	-2.655705	-1.882435
H	-3.915027	-1.260924	-2.709252
H	-5.028719	-1.213159	0.138095
H	-3.663332	0.143091	1.545470
H	-3.559561	0.951323	-1.423814
H	-4.844537	1.364570	-0.316043
C	-1.287865	-1.016663	2.444978
H	-1.666087	-0.130206	2.952523
H	-0.269487	-1.309460	2.698774
C	-2.221438	-2.052075	2.124340
H	-3.265646	-1.857931	2.353872
H	-1.922774	-3.079529	2.311187
H	-0.539843	1.990918	-2.141299
H	-0.660481	2.858902	1.892802
H	-1.315958	3.060182	-0.961014
H	0.632787	1.762767	2.405539
H	0.415128	3.238239	-1.299798
H	1.003169	3.154268	1.352246
H	3.339822	-3.271929	-0.795606
O	2.739902	-1.253779	-0.609575
O	0.445775	-3.884114	-0.126364
C	1.176468	-5.098548	-0.311735
H	1.994659	-5.170291	0.413851
H	0.470072	-5.91082	-0.151817
H	1.580787	-5.15356	-1.328905

L73 – Hexene (PNCN_U_PCF3_X-H-TS1)
Electronic Energy: -1603.41292153
Enthalpy: -1603.103656
Free Energy: -1603.181552

Cr	-1.470371	-0.520941	-0.426188
P	-0.152164	1.390578	0.244114
N	1.454580	0.817567	0.185018
C	1.596951	-0.469361	-0.252520
N	0.548566	-1.214617	-0.519778
H	2.276763	1.385560	0.356347
C	-0.259211	2.164102	1.953063
C	-0.033467	2.942480	-0.811822
C	1.052101	-2.471223	-0.961287
C	2.884126	-1.179742	-0.489525
C	2.391551	-2.507147	-0.962214
H	-2.744645	-1.472737	-0.804317
H	-2.590235	1.395849	-1.901689
H	-3.158841	1.621054	-0.180287
C	-3.565649	-0.346282	-1.013511
C	-2.877041	0.916562	-0.964718
C	-4.567090	-0.686677	0.082285
H	-4.330518	-0.081675	0.969740
H	-5.563116	-0.367897	-0.245923
C	-4.577203	-2.160683	0.476066
H	-4.851000	-2.776847	-0.391951
H	-5.355359	-2.328569	1.226285
C	-3.226163	-2.616509	1.020967

H	-2.957844	-1.978479	1.878485
H	-3.304787	-3.632502	1.428272
C	-2.106793	-2.572111	-0.012738
H	-1.136968	-2.796952	0.444180
H	-2.266446	-3.300040	-0.817514
H	-3.845491	-0.698218	-2.011596
H	3.501772	-0.655014	-1.228859
H	3.489650	-1.231998	0.423805
F	-0.219952	1.187889	2.868894
F	-1.415023	2.825260	2.071863
F	0.751234	3.007341	2.192400
F	0.020247	2.576053	-2.100763
F	1.067495	3.653806	-0.535472
F	-1.107524	3.712503	-0.623445
H	0.345279	-3.239810	-1.243653
H	3.024641	-3.332253	-1.253455

L73 – Octene (PNCN_U_PCF3_X-H-TS2)
Electronic Energy: -1682.02135151
Enthalpy: -1681.650315
Free Energy: -1681.731218

Cr	-1.359425	-0.562223	0.350951
P	0.038694	1.395932	0.120179
N	1.548732	0.794054	-0.380475
C	1.679051	-0.568398	-0.452626
N	0.670406	-1.367694	-0.209246
H	2.349666	1.380686	-0.585917
C	0.491224	2.453763	1.608274
C	-0.280373	2.760657	-1.133780
C	1.170772	-2.688930	-0.363092
C	2.937798	-1.298607	-0.778916
C	2.470757	-2.712772	-0.690954
C	-2.300343	-2.493755	0.367786
C	-2.539599	-2.016657	-1.074707
C	-4.005380	-1.839719	-1.442178
C	-4.745692	-0.819497	-0.588539
C	-3.016768	0.692287	0.541432
C	-4.080996	0.556014	-0.537665
H	-3.221416	-2.927233	0.751585
H	-2.021891	-1.064683	-1.390871
H	-4.495706	-2.817343	-1.370843
H	-5.764895	-0.731427	-0.977693
H	-2.696160	1.741259	0.613591
H	-1.509052	-3.243130	0.407701
H	-2.038774	-2.730042	-1.738671
H	-4.854461	-1.200000	0.438393
H	-3.447690	0.449505	1.523619
H	-3.668559	0.805745	-1.528570
H	-4.856966	1.313380	-0.358845
C	-1.070966	-0.658090	2.381938
H	-1.430395	0.282522	2.796589
H	-0.043934	-0.923943	2.628127
C	-2.012336	-1.718166	2.222199
H	-3.052572	-1.497068	2.446546
H	-1.707171	-2.718202	2.515512
H	3.733529	-1.054566	-0.064211
H	3.328286	-1.025748	-1.766946
F	-0.610888	2.962274	2.164855
F	1.315018	3.458252	1.276128
F	-1.030572	3.720309	-0.584120
F	-0.936153	2.246771	-2.183864
F	0.862175	3.302982	-1.575978
F	1.114161	1.680070	2.507059
H	-4.062287	-1.542994	-2.496272
H	0.496970	-3.522444	-0.212106

H	3.088157	-3.581160	-0.867737

L74 – Hexene (PNCN_U_PCpO_X-H-TS1)
Electronic Energy: -1157.312729
Enthalpy: -1156.970915
Free Energy: -1156.038260

Cr	-1.791693	-0.802604	-0.444986
p	-1.042829	1.103273	0.819800
N	0.622329	0.734192	1.086181
C	1.065071	-0.432857	0.545285
N	0.249736	-1.243632	-0.096799
H	1.298704	1.364385	1.500995
C	1.038914	-2.340510	-0.540364
C	2.465222	-0.945276	0.581639
C	2.323626	-2.222479	-0.177929
H	-2.788724	-1.818169	-1.252918
H	-2.819878	1.227118	-1.819740
H	-3.803837	1.029310	-0.294075
C	-3.689142	-0.760403	-1.519020
C	-3.236485	0.536639	-1.085608
C	-4.879868	-1.393755	-0.807156
H	-5.003979	-0.892841	0.163463
H	-5.786641	-1.171222	-1.381603
C	-4.750071	-2.894860	-0.569932
H	-4.693537	-3.425101	-1.531193
H	-5.655069	-3.258996	-0.074118
C	-3.521853	-3.234859	0.270166
H	-3.561343	-2.654733	1.207241
H	-3.551692	-4.287668	0.578854
C	-2.208382	-2.948347	-0.448589
H	-1.349729	-3.133566	0.206126
H	-2.086688	-3.580670	-1.336441
H	-3.654105	-0.943204	-2.597640
H	3.163564	-0.235648	0.121491
H	2.811858	-1.081489	1.613804
H	3.129467	-2.909704	-0.388990
H	0.557508	-3.128758	-1.104034
O	-1.746495	1.406725	2.259556
O	-0.936731	2.665922	0.343817
C	-1.642974	3.528298	1.266276
C	-1.594868	2.810190	2.595131
H	-0.637608	2.953111	3.110646
H	-2.410315	3.075163	3.267507
H	-1.12967	4.490673	1.274545
H	-2.669065	3.665566	0.908167

L74 – Octene (PNCN_U_PCpO_X-H-TS2)
Electronic Energy: -1235.91897840
Enthalpy: -1235.515918
Free Energy: -1235.589022

Cr	-1.355300	-0.493626	0.308496
P	0.010882	1.488864	0.097965
N	1.579523	0.820140	-0.134581
C	1.689218	-0.529065	-0.303950
N	0.648919	-1.326423	-0.222349
H	2.427121	1.374761	-0.165900
C	1.142708	-2.640391	-0.430173
C	2.961963	-1.264956	-0.567098
C	2.468282	-2.671210	-0.631130
C	-2.274012	-2.443085	0.355960
C	-2.551375	-1.964219	-1.080482
C	-4.027113	-1.811764	-1.420756
C	-4.775533	-0.814172	-0.547358
C	-3.044480	0.690231	0.576874

C	-4.130921	0.570263	-0.481773
H	-3.187780	-2.867213	0.767237
H	-2.059206	-1.002196	-1.405880
H	-4.497555	-2.799355	-1.351044
H	-5.799810	-0.737958	-0.926369
H	-2.724824	1.738807	0.667487
H	-1.492987	-3.202832	0.365315
H	-2.053731	-2.666025	-1.758851
H	-4.106439	-1.507038	-2.471327
H	-4.868040	-1.210329	0.475222
H	-3.456798	0.419288	1.560127
H	-3.740148	0.843217	-1.475331
H	-4.916380	1.311065	-0.275103
C	-0.995926	-0.577547	2.328102
H	-1.383576	0.342675	2.761018
H	0.048944	-0.796713	2.543323
C	-1.893927	-1.680981	2.194714
H	-2.928735	-1.509696	2.478001
H	-1.528047	-2.667865	2.462590
H	3.694386	-1.092591	0.231467
H	3.440768	-0.925753	-1.493850
C	0.064755	3.915438	0.847946
C	0.295185	3.881248	-0.646246
H	0.767769	4.559449	1.377859
H	-0.959746	4.207776	1.100130
H	1.360094	3.930057	-0.905601
H	-0.241074	4.659211	-1.189071
O	-0.238688	2.603095	-1.070422
O	0.286192	2.558935	1.303098
H	0.445708	-3.468813	-0.410777
H	3.085609	-3.538952	-0.811092

L75 – Hexene (PNCN_U_PMe_X-H_TS1)
Electronic Energy: -1008.08352137
Enthalpy: -1007.732272
Free Energy: -1007.799102

Cr	-1.440628	-0.507214	-0.426005
P	-0.137469	1.455849	0.229199
N	1.476686	0.809962	0.185393
C	1.606741	-0.483036	-0.185890
N	0.554709	-1.231522	-0.458777
H	2.313657	1.351254	0.362109
C	-0.282010	2.152231	1.900502
C	-0.024327	2.929912	-0.824262
C	1.057851	-2.511256	-0.819433
C	2.892148	-1.228701	-0.339228
C	2.395885	-2.570442	-0.768568
H	-2.717371	-1.477940	-0.760779
H	-2.569411	1.378976	-1.930215
H	-3.153249	1.620100	-0.218012
C	-3.533297	-0.361223	-1.027095
C	-2.849406	0.907659	-0.987124
H	0.767630	3.606277	-0.490550
H	-1.242072	2.668088	1.991901
C	-4.558991	-0.681533	0.052656
H	-4.335468	-0.065391	0.936388
H	-5.548677	-0.363982	-0.296413
C	-4.581510	-2.149319	0.468785
H	-4.831072	-2.777549	-0.398145
H	-5.381171	-2.307038	1.198987
C	-3.245948	-2.597666	1.056925
H	-3.004995	-1.946648	1.912785
H	-3.338292	-3.608005	1.475868
C	-2.094952	-2.560021	0.055588
H	-1.140768	-2.768911	0.550518

H	-2.222527	-3.312353	-0.732926
H	-3.799097	-0.731048	-2.022654
H	-0.249938	1.358916	2.649977
H	0.514055	2.873492	2.105583
H	0.163295	2.642615	-1.860978
H	-0.974415	3.469835	-0.787234
H	3.545776	-0.746928	-1.076892
H	3.458519	-1.246470	0.599960
H	3.023552	-3.419025	-0.997509
H	0.352475	-3.285148	-1.092509

L75 – Octene (PNCN_U_PMe_X-H_TS2)
Electronic Energy: -1086.69081203
Enthalpy: -1086.278421
Free Energy: -1086.350018

Cr	-1.318815	-0.536554	0.479754
P	0.021686	1.471346	0.108474
N	1.552333	0.777148	-0.323340
C	1.681386	-0.573162	-0.301981
N	0.675076	-1.369016	-0.009125
H	2.370140	1.331267	-0.544529
C	0.407732	2.569030	1.499980
C	-0.343350	2.605463	-1.260148
C	1.193759	-2.688653	-0.045957
C	2.945311	-1.323329	-0.580120
C	2.494016	-2.730519	-0.371682
C	-2.280838	-2.477600	0.307626
C	-2.418111	-1.900786	-1.114134
C	-3.852849	-1.682288	-1.573480
C	-4.663573	-0.727638	-0.707849
C	-3.021621	0.653282	0.670231
C	-4.009494	0.636282	-0.487860
H	-3.238953	-2.901568	0.601982
H	-1.862996	-0.943515	-1.333441
H	-4.349176	-2.658920	-1.615861
H	-5.647104	-0.606118	-1.173533
H	-2.711908	1.686974	0.887590
H	-1.528205	-3.265171	0.319887
H	-1.886125	-2.581410	-1.788152
H	-3.829832	-1.306950	-2.604093
H	-4.856646	-1.186883	0.273428
H	-3.530344	0.307396	1.583157
H	-3.526681	0.964804	-1.424004
H	-4.801223	1.376871	-0.304750
C	-1.144694	-0.783469	2.495569
H	-1.560168	0.104317	2.970195
H	-0.119770	-1.031364	2.770021
C	-2.040259	-1.863102	2.205855
H	-3.091748	-1.696518	2.424743
H	-1.709936	-2.871922	2.437911
H	-0.499228	2.043011	-2.183579
H	0.791037	1.983922	2.338764
H	-1.263678	3.152307	-1.035584
H	1.139788	3.334206	1.226833
H	3.752143	-1.016596	0.096298
H	3.312519	-1.127513	-1.595301
H	0.457839	3.333565	-1.415056
H	-0.508759	3.069688	1.825587
H	3.120372	-3.604896	-0.469934
H	0.534115	-3.514380	0.190337

L76 – Hexene (PNCN_U_PPh_X-H_TS1)
Electronic Energy: -1391.52430484
Enthalpy: -1391.059630
Free Energy: -1391.140851

Cr	-1.342894	-0.421431	-0.459166
P	-0.005417	1.522846	0.176795
N	1.594989	0.837071	0.197123
C	1.692917	-0.479074	-0.098771
N	0.632190	-1.197652	-0.414259
H	2.423477	1.332488	0.503258
C	1.105904	-2.505762	-0.703339
C	2.954172	-1.279392	-0.139228
C	2.434360	-2.614147	-0.561781
H	-2.648379	-1.354890	-0.769736
H	-2.417416	1.526362	-1.927632
H	-3.031836	1.707205	-0.217841
C	-3.419407	-0.237861	-1.108005
C	-2.725851	1.022722	-1.011465
C	-4.518257	-0.571567	-0.106126
H	-4.347641	0.016779	0.807850
H	-5.477642	-0.229924	-0.511625
C	-4.585757	-2.052004	0.259284
H	-4.764964	-2.648202	-0.646983
H	-5.445923	-2.227694	0.912631
C	-3.308764	-2.533018	0.945838
H	-3.153698	-1.928214	1.852609
H	-3.441302	-3.562909	1.301325
C	-2.064764	-2.452331	0.061735
H	-1.158628	-2.637241	0.649788
H	-2.092923	-3.204035	-0.737272
H	-3.624312	-0.589049	-2.124719
H	3.676705	-0.846055	-0.841625
H	3.452737	-1.291371	0.837909
C	-0.375078	1.985939	1.887999
C	-1.146070	1.082446	2.632178
C	0.095655	3.157999	2.493399
C	-1.440356	1.340702	3.966117
H	-1.513855	0.171480	2.151460
C	-0.202383	3.413942	3.827462
H	0.682234	3.870955	1.918668
C	-0.967465	2.508510	4.561312
H	-2.040350	0.639014	4.537205
H	0.161343	4.323189	4.296207
H	-1.199862	2.717070	5.601260
C	0.214062	3.064198	-0.742348
C	-0.726160	4.091924	-0.578152
C	1.223077	3.199299	-1.703615
C	-0.644984	5.241374	-1.356232
H	-1.515429	3.997458	0.164402
C	1.301022	4.355744	-2.473609
H	1.948722	2.403436	-1.849441
C	0.368356	5.375547	-2.302792
H	-1.373971	6.034197	-1.219829
H	2.091256	4.457678	-3.211229
H	0.429779	6.275059	-2.907544
H	3.041056	-3.493659	-0.719459
H	0.389060	-3.261069	-0.997480

L76 – Octene (PNCN_U_PPh_X-H_TS2)
Electronic Energy: -1470.13065837
Enthalpy: -1469.604985
Free Energy: -1469.691425

Cr	-1.251775	-0.515539	0.649503
P	0.068507	1.520061	0.160532
N	1.565916	0.792802	-0.350150
C	1.741146	-0.538404	-0.152615
N	0.767382	-1.317758	0.264512
H	2.370782	1.343001	-0.624479

C	1.317551	-2.620784	0.363115
C	3.014393	-1.287206	-0.387546
C	2.606953	-2.671512	-0.003437
C	-2.149101	-2.396922	0.006163
C	-2.100964	-1.588817	-1.300010
C	-3.458201	-1.277170	-1.913995
C	-4.392591	-0.477982	-1.015925
C	-2.968693	0.660097	0.772506
C	-3.795501	0.829580	-0.494156
H	-3.121743	-2.880054	0.081366
H	-1.542046	-0.611847	-1.267649
H	-3.931285	-2.223896	-2.200518
H	-5.309474	-0.277149	-1.580242
H	-2.674008	1.642862	1.172777
H	-1.370676	-3.159968	0.006961
H	-1.464362	-2.145301	-1.997604
H	-3.291414	-0.722409	-2.846782
H	-4.702871	-1.095149	-0.158956
H	-3.593182	0.200254	1.553898
H	-3.198926	1.300967	-1.292468
H	-4.616227	1.536096	-0.302314
C	-1.394518	-1.111317	2.597540
H	-1.884109	-0.310961	3.149818
H	-0.423188	-1.425470	2.979138
C	-2.232835	-2.100008	1.989889
H	-3.305761	-1.940066	2.061389
H	-1.950634	-3.143782	2.100045
H	3.834255	-0.888127	0.221923
H	3.342951	-1.197260	-1.430458
C	0.523609	2.739825	1.412679
C	0.241677	2.443902	2.752375
C	1.191850	3.928591	1.086102
C	0.625989	3.327603	3.755831
H	-0.281511	1.522128	3.000643
C	1.576914	4.804450	2.094055
H	1.398361	4.169431	0.045429
C	1.293980	4.504129	3.426346
H	0.401214	3.099413	4.793049
H	2.095278	5.724462	1.841537
H	1.593045	5.193634	4.210056
C	-0.478308	2.438839	-1.299425
C	-1.208531	3.626049	-1.159414
C	-0.333797	1.861991	-2.569203
C	-1.768543	4.234083	-2.279509
H	-1.339128	4.075771	-0.178042
C	-0.894101	2.476601	-3.683378
H	0.225713	0.935966	-2.686043
C	-1.612623	3.662251	-3.539368
H	-2.327140	5.157878	-2.164831
H	-0.768273	2.030412	-4.665382
H	-2.051277	4.139659	-4.410190
H	3.254551	-3.535900	-0.017780
H	0.685002	-3.424822	0.720363

L77 – Hexene
Electronic Energy: -1322.60371887
Enthalpy: -1322.010619
Free Energy: -1322.095434

N	1.238142	1.441242	-0.137747
C	1.663014	0.298844	-0.728458
N	0.827551	-0.648941	-1.064683
P	-0.476817	1.636825	0.074554
H	1.927048	2.149102	0.086575
C	-0.693860	1.767242	1.905459
C	0.221580	2.788418	2.563908

H	1.274454	2.501103	2.460870
H	0.098880	3.795108	2.152538
H	0.012438	2.849113	3.636098
C	-0.767981	3.323277	-0.619567
C	1.613062	-1.723834	-1.704853
C	3.100810	0.012183	-1.066302
C	3.036032	-1.524902	-1.178792
H	1.552117	-1.612382	-2.795262
C	-0.585519	3.295778	-2.132256
H	-1.334092	2.655316	-2.611376
H	-0.702997	4.301785	-2.545272
H	0.404349	2.935117	-2.426433
H	0.007310	3.965890	-0.176242
C	-2.139653	3.855287	-0.221833
H	-2.251682	3.973307	0.859659
H	-2.296915	4.839854	-0.671572
H	-2.945111	3.205255	-0.579117
H	-1.739955	2.082936	2.026007
C	-0.542294	0.375027	2.510072
H	-1.237442	-0.344188	2.052842
H	0.473474	-0.015743	2.376137
H	-0.746312	0.392043	3.584702
H	1.196973	-2.702485	-1.448092
C	3.200177	-2.203853	0.185013
C	4.160910	0.574126	-0.124818
C	4.199385	-0.150729	1.213210
C	4.359234	-1.650721	1.001114
H	2.270320	-2.064198	0.759557
H	3.300914	-3.284280	0.035751
H	5.135515	0.470569	-0.616528
H	4.018185	1.655001	0.009815
H	5.012766	0.246663	1.828274
H	3.268477	0.042579	1.769430
H	5.308314	-1.843855	0.481729
H	4.423205	-2.171554	1.961830
H	3.258712	0.432083	-2.072040
H	3.792826	-1.895719	-1.877937
Cr	-1.237322	-0.576554	-0.623132
H	-2.182129	-1.912205	-0.694430
H	-3.255179	0.880031	-1.608495
H	-3.460236	0.810985	0.203039
C	-3.347295	-1.131515	-0.765822
C	-3.127402	0.293127	-0.698568
C	-4.004251	-1.846377	0.408545
H	-3.836260	-1.249616	1.317811
H	-5.088761	-1.856979	0.248480
C	-3.480078	-3.260908	0.637246
H	-3.641301	-3.864904	-0.267329
H	-4.060029	-3.742038	1.430768
C	-1.997778	-3.266520	1.004556
H	-1.864238	-2.660942	1.914070
H	-1.684867	-4.282063	1.279208
C	-1.084327	-2.729531	-0.096119
H	-0.073586	-2.555053	0.293106
H	-0.997606	-3.436607	-0.930353
H	-3.652058	-1.516732	-1.744365

L77 – Octene

Electronic Energy: -1401.21025173
Enthalpy: -1400.556187
Free Energy: -1400.646273

N	1.276616	1.118820	-0.828323
C	1.592232	-0.200080	-0.909057
N	0.787754	-1.128993	-0.475991
P	-0.166499	1.596607	0.012704

H	1.958620	1.787652	-1.165556
C	0.470564	2.661075	1.385388
C	1.310614	3.829034	0.886012
H	2.215922	3.481085	0.373302
H	0.764243	4.490709	0.207893
H	1.644789	4.437556	1.731448
C	-0.963898	2.755823	-1.186185
C	1.464817	-2.425254	-0.651937
C	2.875788	-0.717400	-1.506718
C	2.951158	-2.079957	-0.788249
H	1.069091	-2.931825	-1.544143
Cr	-1.136908	-0.666299	0.452391
C	-1.881518	-2.653810	-0.062222
C	-2.385115	-1.821428	-1.244261
C	-3.900348	-1.729668	-1.365470
C	-4.612064	-1.148336	-0.151019
C	-2.899235	0.179037	1.193375
C	-4.111935	0.231930	0.275612
H	-2.682399	-3.307627	0.277960
H	-1.987005	-0.771503	-1.316340
H	-4.284947	-2.735132	-1.573694
H	-5.682695	-1.109633	-0.378485
H	-2.654216	1.186176	1.565284
H	-1.020265	-3.257680	-0.348590
H	-1.942275	-2.246629	-2.152937
H	-4.139904	-1.123850	-2.249017
H	-4.516243	-1.837407	0.701932
H	-3.159216	-0.405588	2.089285
H	-3.901211	0.832707	-0.625442
H	-4.933853	0.761891	0.779674
C	-0.582496	-1.339089	2.315859
H	-1.001233	-0.636488	3.034147
H	0.496661	-1.482005	2.361287
C	-1.393825	-2.437352	1.912411
H	-2.410857	-2.469341	2.294325
H	-0.933535	-3.417615	1.824723
C	-1.484644	1.982865	-2.390828
H	-2.320168	1.331754	-2.104982
H	-1.860464	2.673117	-3.151903
H	-0.712327	1.364461	-2.859143
H	-0.172574	3.443953	-1.517872
C	-2.073402	3.551072	-0.507381
H	-1.706685	4.182344	0.307095
H	-2.558221	4.208891	-1.234453
H	-2.847456	2.889532	-0.101599
H	-0.437919	3.048733	1.867342
C	1.225106	1.803535	2.393650
H	0.584901	1.038581	2.840004
H	2.081522	1.297437	1.931149
H	1.615676	2.426429	3.203465
H	1.257517	-3.070655	0.210834
C	3.606406	-1.951879	0.590506
C	4.114707	0.165170	-1.403970
C	4.668536	0.239352	0.011704
C	4.905287	-1.159468	0.565230
H	2.902036	-1.443202	1.267856
H	3.760011	-2.952527	1.008779
H	4.881040	-0.254910	-2.066499
H	3.906431	1.165351	-1.807567
H	5.592274	0.825969	0.020062
H	3.957192	0.772178	0.662793
H	5.647447	-1.676550	-0.059090
H	5.332867	-1.107878	1.571391
H	2.656016	-0.894546	-2.570945
H	3.493695	-2.811667	-1.396206

L78 – Hexene
Electronic Energy: -1660.70545150
Enthalpy: -1660.063191
Free Energy: -1660.165356

N	-0.402367	-1.851930	0.429761
C	-1.124815	-0.692163	0.357721
N	-0.452887	0.435731	0.308697
H	-0.912195	-2.718473	0.553854
C	-1.093769	1.684510	0.035434
C	-1.328507	2.599005	1.076142
C	-1.336075	2.027121	-1.310400
C	-1.825441	3.862850	0.743816
C	-1.831566	3.298586	-1.595355
C	-2.073281	4.215535	-0.576206
H	-2.014908	4.575566	1.543211
H	-2.025654	3.568019	-2.630761
H	-2.454200	5.204267	-0.813581
C	-2.588952	-0.844813	0.256413
C	-3.485258	-0.001764	0.927687
C	-3.107720	-1.871662	-0.547165
C	-4.852585	-0.187449	0.796460
C	-4.478931	-2.035444	-0.688199
C	-5.377772	-1.199233	-0.018342
H	-3.111987	0.782181	1.576492
H	-2.430101	-2.523558	-1.095424
H	-5.532545	0.466143	1.337148
H	-4.861287	-2.824543	-1.330556
C	-1.094894	2.242571	2.513669
H	-0.502439	1.330632	2.626285
H	-0.582166	3.049987	3.044704
H	-2.040385	2.078962	3.046130
C	-1.064111	1.042970	-2.406839
H	-1.684235	0.142050	-2.318279
H	-1.254116	1.480494	-3.389092
H	-0.018441	0.697615	-2.401738
C	-6.854807	-1.368625	-0.167805
H	-7.105941	-2.259539	-0.747335
H	-7.349947	-1.448392	0.804870
H	-7.302621	-0.506859	-0.674145
C	2.378427	-3.845879	1.371393
C	2.497107	-4.132997	-0.111483
H	1.515897	-4.373387	1.811741
H	3.275017	-4.137583	1.925871
H	2.257109	-5.174074	-0.351787
H	3.516621	-3.925124	-0.473980
P	1.317673	-1.812880	0.133447
N	1.517972	-3.245578	-0.736857
N	2.206506	-2.393156	1.440153
C	1.399537	-3.271683	-2.181389
H	2.344352	-3.040821	-2.693634
H	1.068707	-4.263196	-2.506414
H	0.644003	-2.548916	-2.507227
C	2.055334	-1.787876	2.749166
H	1.167341	-2.153242	3.285939
H	2.938781	-1.996249	3.358966
H	1.966531	-0.700495	2.647261
Cr	1.592636	0.518472	-0.333700
H	2.406525	1.916326	-0.622049
H	2.463060	-0.404347	-2.682351
H	3.691686	-0.848656	-1.408102
C	3.253025	1.279757	-1.534007
C	2.960513	-0.116826	-1.755620
C	4.529371	1.655443	-0.789471
H	4.843105	0.790762	-0.186126
H	5.327482	1.820528	-1.522659

C	4.380224	2.866555	0.126495
H	4.076219	3.744147	-0.462011
H	5.352859	3.114168	0.562884
C	3.361108	2.614855	1.235799
H	3.676003	1.721007	1.797610
H	3.381159	3.439431	1.960645
C	1.940416	2.415808	0.719876
H	1.273958	2.066431	1.516299
H	1.508396	3.341738	0.320942
H	2.995977	1.956497	-2.355539

L78 – Octene
Electronic Energy: -1739.31328513
Enthalpy: -1738.609459
Free Energy: -1738.714264

N	0.450240	1.866551	0.400149
C	1.200124	0.718176	0.347490
N	0.577521	-0.434722	0.404327
H	0.946335	2.742082	0.517244
C	1.286226	-1.635045	0.104456
C	1.528183	-2.559191	1.137507
C	1.648127	-1.920904	-1.225992
C	2.148139	-3.768841	0.821963
C	2.267907	-3.143714	-1.497275
C	2.518095	-4.063964	-0.486356
H	2.344396	-4.481014	1.619886
H	2.549346	-3.369878	-2.523112
H	2.999411	-5.009560	-0.716969
C	2.656923	0.925198	0.194845
C	3.599829	0.130178	0.857788
C	3.121516	1.964609	-0.628634
C	4.957837	0.372861	0.702798
C	4.479776	2.187697	-0.791733
C	5.426076	1.397538	-0.126123
H	3.273496	-0.668443	1.514934
H	2.408256	2.582221	-1.170956
H	5.673330	-0.245708	1.238367
H	4.817592	2.987332	-1.446511
C	1.156018	-2.225547	2.547504
H	0.098081	-1.957517	2.630771
H	1.349792	-3.063646	3.220785
H	1.710584	-1.358506	2.928728
C	1.361839	-0.952483	-2.330697
H	2.018211	-0.073415	-2.296204
H	1.498482	-1.419667	-3.308814
H	0.333497	-0.572967	-2.279566
C	6.888802	1.645651	-0.305429
Cr	-1.720020	-0.531024	0.445173
C	-1.887909	-2.703658	0.481236
C	-1.767397	-2.415474	-1.015317
C	-2.976401	-2.795656	-1.857999
C	-4.284831	-2.132796	-1.450317
C	-3.713707	-0.099348	-0.018064
C	-4.221089	-0.608955	-1.358006
H	-2.708832	-3.396355	0.656438
H	-1.500983	-1.355690	-1.298842
H	-3.085217	-3.885813	-1.821267
H	-5.052701	-2.437002	-2.169560
H	-3.848560	0.990144	0.042967
H	-0.958738	-3.121415	0.870553
H	-0.860215	-2.921540	-1.367814
H	-2.755261	-2.546712	-2.903834
H	-4.616662	-2.529668	-0.479168
H	-4.325976	-0.526912	0.789341
H	-3.610912	-0.212278	-2.186871

H	-5.228908	-0.207061	-1.536803
C	-2.121633	-0.416549	2.471694
H	-2.925255	0.306818	2.588365
H	-1.204870	-0.205155	3.023789
C	-2.484093	-1.771613	2.247860
H	-3.541123	-1.994582	2.135517
H	-1.924785	-2.557546	2.747059
H	7.150094	2.683622	-0.076201
H	7.492468	0.998106	0.333964
H	7.196813	1.469523	-1.341520
C	-2.444804	4.178750	0.257282
C	-1.844238	4.034042	-1.124289
H	-2.281545	5.174831	0.681692
H	-3.529587	3.988908	0.235356
H	-0.871500	4.550422	-1.195082
H	-2.496876	4.431557	-1.907072
P	-1.273566	1.839830	0.162507
N	-1.702911	2.587862	-1.287768
N	-1.745896	3.184505	1.073057
C	-1.206311	2.088108	-2.550881
H	-1.833345	2.458754	-3.366748
H	-0.164259	2.380898	-2.756274
H	-1.260058	0.993791	-2.562125
C	-2.156594	3.064980	2.458391
H	-2.045239	4.035164	2.951788
H	-3.202928	2.743972	2.570300
H	-1.513009	2.353350	2.981162

L79 – Hexene

Electronic Energy: -1700.01930423
Enthalpy: -1699.347387
Free Energy: -1699.453217

N	1.262884	-0.596232	0.256047
C	0.871573	0.704039	0.287888
N	-0.406997	0.970886	0.191321
H	2.254982	-0.789956	0.352203
C	-0.886008	2.311386	0.301904
C	-0.846964	3.184250	-0.799456
C	-1.516031	2.679306	1.507748
C	-1.446374	4.441081	-0.665090
C	-2.095603	3.943918	1.597834
C	-2.065223	4.821600	0.517758
H	-1.425332	5.122794	-1.512177
H	-2.578420	4.236839	2.527006
H	-2.526724	5.800974	0.599712
C	-0.184041	2.809251	-2.090593
H	-0.050392	1.728432	-2.196858
H	-0.766211	3.160454	-2.947102
H	0.808034	3.269002	-2.184956
C	-1.583439	1.725625	2.663983
H	-0.610693	1.280100	2.901064
H	-1.949184	2.223889	3.564636
H	-2.271279	0.884907	2.474835
C	1.199214	-3.853276	-0.937967
C	0.935697	-4.279353	0.490510
H	2.234174	-3.491102	-1.060374
H	1.036469	-4.664664	-1.652967
H	1.791920	-4.799752	0.932378
H	0.061036	-4.946582	0.548819
P	0.033527	-1.843652	0.215009
N	0.690054	-3.030462	1.214107
N	0.228064	-2.780956	-1.175714
C	0.318180	-3.133665	2.612834
H	-0.580204	-3.747741	2.767548
H	1.139929	-3.581397	3.179990

H	0.133962	-2.138699	3.028637
C	0.271537	-2.119940	-2.466961
H	1.225422	-1.599709	-2.648478
H	0.119750	-2.853761	-3.262718
H	-0.536041	-1.382297	-2.534175
C	1.931584	1.760798	0.486566
H	1.661685	2.624563	-0.128753
H	1.838211	2.110469	1.523505
C	3.337321	1.311719	0.202214
C	3.819044	1.273373	-1.111861
C	4.179340	0.880704	1.230221
C	5.106692	0.830264	-1.383214
H	3.177719	1.601559	-1.928706
C	5.469642	0.435554	0.953884
H	3.824669	0.904554	2.259070
C	5.958237	0.405225	-0.354758
H	5.465241	0.816220	-2.410085
H	6.112962	0.112754	1.769194
C	7.352917	-0.047588	-0.653327
H	7.381270	-0.744179	-1.496753
H	7.995648	0.797119	-0.924696
H	7.811778	-0.541093	0.206673
Cr	-1.935948	-0.485119	0.238861
H	-3.523192	-0.165552	-0.026209
H	-2.622576	-1.988032	2.327989
H	-2.609286	-3.057869	0.847932
C	-3.904782	-1.315394	0.689529
C	-2.810749	-2.066198	1.256400
C	-4.686644	-1.910739	-0.475352
H	-4.044926	-2.647959	-0.980840
H	-5.539957	-2.472188	-0.076809
C	-5.151950	-0.877955	-1.498389
H	-5.798110	-0.134941	-1.009109
H	-5.772147	-1.369147	-2.254713
C	-3.976588	-0.171650	-2.172223
H	-3.340646	-0.936959	-2.644119
H	-4.339371	0.458116	-2.994995
C	-3.136905	0.666719	-1.212767
H	-2.213524	1.016425	-1.689699
H	-3.672816	1.560663	-0.869680
H	-4.520098	-0.755605	1.401767

L79 – Octene

Electronic Energy: -1778.62491536
Enthalpy: -1777.891307
Free Energy: -1777.998599

N	-1.346556	-0.508207	0.266398
C	-0.927926	0.786325	0.184290
N	0.352290	1.049633	0.185860
H	-2.349882	-0.667246	0.264611
C	0.759132	2.404810	-0.010587
C	1.017077	3.226372	1.101439
C	0.957798	2.874913	-1.322870
C	1.496425	4.519029	0.878155
C	1.443540	4.172981	-1.500776
C	1.717290	4.990923	-0.410912
H	1.696854	5.157497	1.735176
H	1.601529	4.538852	-2.512558
H	2.095424	5.996888	-0.565308
C	0.782232	2.727205	2.492133
H	1.430835	1.878152	2.733985
H	0.973875	3.509165	3.230200
H	-0.245690	2.375865	2.641220
C	0.630528	2.015516	-2.504935
H	-0.451545	1.864995	-2.619500

H	0.990905	2.464967	-3.433090
H	1.068270	1.014438	-2.420192
Cr	1.869802	-0.634433	0.449745
C	3.563524	0.711229	0.580820
C	3.476128	0.453808	-0.921964
C	4.684758	-0.238358	-1.534387
C	4.984523	-1.615669	-0.958972
C	2.887676	-2.448135	0.239491
C	3.794695	-2.575701	-0.974985
H	4.597291	0.629003	0.910186
H	2.576572	-0.133078	-1.273262
H	5.553740	0.418199	-1.411185
H	5.822338	-2.040501	-1.521808
H	2.136888	-3.252112	0.230006
H	3.167181	1.695725	0.837712
H	3.270181	1.415075	-1.408458
H	4.518304	-0.326451	-2.615445
H	5.344018	-1.517221	0.076351
H	3.479010	-2.593782	1.155535
H	3.219873	-2.439021	-1.906500
H	4.177987	-3.604872	-1.032187
C	1.815773	-0.865730	2.510080
H	1.801975	-1.937439	2.693473
H	0.993874	-0.295461	2.943623
C	3.083669	-0.241211	2.380999
H	3.962386	-0.879588	2.402751
H	3.243647	0.734535	2.830376
C	-1.298261	-4.204705	0.083050
C	-1.532809	-3.610707	-1.288286
H	-2.188229	-4.706820	0.476719
H	-0.473509	-4.934259	0.061175
H	-2.539382	-3.163988	-1.362653
H	-1.428511	-4.349435	-2.088327
P	-0.216882	-1.823741	0.066266
N	-0.484763	-2.595294	-1.413904
N	-0.972105	-3.058140	0.932505
C	-0.454676	-1.822095	-2.638638
H	-0.378395	-2.495733	-3.496337
H	-1.349275	-1.191514	-2.771959
H	0.427277	-1.172063	-2.647485
C	-0.666728	-3.327733	2.323747
H	-1.502502	-3.869860	2.776041
H	0.242277	-3.932967	2.455020
H	-0.547490	-2.390201	2.871731
C	-1.989899	1.862370	0.093183
H	-1.844336	2.527637	0.953732
H	-1.747543	2.478848	-0.780462
C	-3.406428	1.371040	0.027163
C	-4.139877	1.138105	1.195350
C	-4.007017	1.079266	-1.201718
C	-5.436158	0.639144	1.134172
H	-3.689252	1.355235	2.162314
C	-5.304920	0.583187	-1.259631
H	-3.452961	1.252438	-2.123471
C	-6.044699	0.356073	-0.093815
H	-5.990888	0.470353	2.054402
H	-5.757618	0.371177	-2.225644
C	-7.453735	-0.143102	-0.158262
H	-7.698307	-0.783370	0.693659
H	-8.168199	0.687913	-0.143459
H	-7.642902	-0.708293	-1.074582

L80 – Hexene

Electronic Energy: -1778.63576635
Enthalpy: -1777.904675
Free Energy: -1778.012417

N	-0.050560	1.743760	0.509021
C	0.541199	0.512628	0.414340
N	-0.245393	-0.535678	0.312342
H	0.537882	2.522797	0.780210
C	0.279779	-1.827248	-0.006105
C	0.424670	-2.802069	0.995512
C	0.516324	-2.130548	-1.362519
C	0.827562	-4.085442	0.613565
C	0.917398	-3.423104	-1.697212
C	1.072266	-4.398796	-0.716576
H	0.947553	-4.844764	1.383017
H	1.107321	-3.661853	-2.740843
H	1.381000	-5.402708	-0.992070
C	2.015030	0.506417	0.355179
C	2.799126	-0.435883	1.033901
C	2.663768	1.473550	-0.424731
C	4.179706	-0.405693	0.922683
C	4.048108	1.480565	-0.545160
C	4.839363	0.541439	0.124171
H	2.328214	-1.175618	1.671259
H	2.076528	2.205647	-0.974909
H	4.762438	-1.142036	1.470361
H	4.511079	2.231691	-1.176801
C	0.197185	-2.497724	2.446334
H	-0.266436	-1.519989	2.601603
H	-0.441792	-3.253261	2.913701
H	1.138565	-2.504576	3.009754
C	0.335710	-1.083677	-2.419861
H	1.030561	-0.243325	-2.294312
H	0.493402	-1.496836	-3.418292
H	-0.677972	-0.652180	-2.403952
C	6.361112	0.512267	0.016740
C	-2.178490	4.448841	-0.048877
C	-3.023914	3.963591	1.109973
P	-1.748758	1.894945	0.145816
N	-1.932634	3.243915	-0.843667
N	-2.451832	2.666314	1.476138
C	-1.140806	3.385746	-2.048266
H	-1.664552	4.023824	-2.766029
H	-0.151428	3.828594	-1.856093
H	-0.989908	2.407586	-2.515785
C	-3.184314	1.873157	2.447117
H	-3.272591	2.425843	3.386609
H	-4.199224	1.612312	2.106135
H	-2.639179	0.947827	2.661981
C	6.970204	0.694422	1.413540
H	6.660566	-0.096320	2.104002
H	8.063212	0.668212	1.354784
H	6.683213	1.654562	1.854453
C	6.896377	1.614167	-0.895077
H	6.518972	1.521939	-1.919076
H	6.641505	2.613789	-0.527202
H	7.987604	1.555342	-0.944862
C	6.797973	-0.846241	-0.548662
H	6.479803	-1.677904	0.087557
H	6.386455	-1.015216	-1.548977
H	7.889442	-0.889600	-0.624827
Cr	-2.283493	-0.382228	-0.332819
H	-3.270108	-1.655220	-0.638661
H	-3.135036	0.779599	-2.575899
H	-4.256696	1.260362	-1.225408
C	-4.058135	-0.891212	-1.500314
C	-3.626138	0.477187	-1.650381
C	-5.348166	-1.178796	-0.739936
H	-5.556160	-0.324942	-0.077693

H	-6.176222	-1.215523	-1.457497
C	-5.303259	-2.453236	0.097886
H	-5.098157	-3.317431	-0.550087
H	-6.287372	-2.632156	0.541969
C	-4.245304	-2.372975	1.196601
H	-4.467168	-1.496927	1.826105
H	-4.330072	-3.241309	1.863081
C	-2.818769	-2.268899	0.665884
H	-2.117257	-2.016875	1.468310
H	-2.472963	-3.207782	0.216284
H	-3.894640	-1.541454	-2.365906
H	-1.234957	4.898658	0.305669
H	-2.698310	5.193806	-0.658389
H	-2.985021	4.644633	1.966445
H	-4.077338	3.855297	0.805363

L80 – Octene
Electronic Energy: -1857.24253986
Enthalpy: -1856.450354
Free Energy: -1856.563885

N	0.051861	1.783166	0.267663
C	0.653832	0.551840	0.324804
N	-0.093865	-0.518672	0.451516
H	0.667127	2.588329	0.239252
C	0.492425	-1.807193	0.263238
C	0.600204	-2.675116	1.366861
C	0.859640	-2.230735	-1.029144
C	1.094392	-3.963324	1.160929
C	1.347457	-3.531241	-1.189515
C	1.467648	-4.394327	-0.108159
H	1.186573	-4.631545	2.013830
H	1.631293	-3.861984	-2.185851
H	1.847263	-5.401256	-0.252518
C	2.125937	0.570449	0.181159
C	2.961881	-0.235283	0.965487
C	2.715230	1.420473	-0.762726
C	4.336453	-0.185250	0.800393
C	4.094648	1.447250	-0.934077
C	4.937884	0.645807	-0.157767
H	2.535537	-0.889956	1.718362
H	2.084653	2.038606	-1.399371
H	4.959518	-0.812927	1.432886
H	4.511789	2.104176	-1.690326
C	0.206835	-2.215390	2.734937
H	-0.850819	-1.932999	2.775081
H	0.371647	-2.997291	3.479767
H	0.765684	-1.327393	3.054742
C	0.732668	-1.327777	-2.216970
H	1.567576	-0.619466	-2.284528
H	0.722825	-1.902182	-3.146749
H	-0.184460	-0.727495	-2.183152
C	6.455615	0.644265	-0.315341
Cr	-2.372411	-0.370824	0.329483
C	-2.760510	-2.503495	0.426001
C	-2.563227	-2.282870	-1.072119
C	-3.777289	-2.605211	-1.930616
C	-5.026395	-1.805878	-1.588870
C	-4.272332	0.264106	-0.288724
C	-4.811639	-0.293591	-1.598285
H	-3.638454	-3.123882	0.593462
H	-2.216846	-1.252110	-1.384128
H	-3.980783	-3.678380	-1.837925
H	-5.810789	-2.082394	-2.301278
H	-4.265218	1.364056	-0.326134
H	-1.883374	-2.970150	0.877479

H	-1.686624	-2.866850	-1.377351
H	-3.514113	-2.433010	-2.981920
H	-5.405149	-2.105868	-0.600373
H	-4.963698	0.005378	0.526345
H	-4.150233	-0.029792	-2.440027
H	-5.769548	0.196276	-1.827636
C	-2.882689	-0.138830	2.329605
H	-3.583594	0.693880	2.357993
H	-1.985599	-0.034498	2.940173
C	-3.393154	-1.444430	2.116586
H	-4.456856	-1.547598	1.922099
H	-2.969578	-2.274132	2.675207
C	-2.601172	4.193327	-0.836712
C	-2.184263	4.463973	0.591129
P	-1.676925	1.949503	0.151463
N	-1.922985	2.947328	-1.191348
N	-2.164513	3.146942	1.236265
C	-2.236600	2.375317	-2.486826
H	-3.311305	2.177657	-2.613807
H	-1.916311	3.057286	-3.280418
H	-1.692498	1.435259	-2.624521
C	-1.688948	3.136265	2.607802
H	-0.691364	3.591586	2.704881
H	-2.382807	3.693913	3.243258
H	-1.631690	2.114596	2.986400
C	7.101596	1.056544	1.014046
H	6.842901	0.371780	1.827512
H	8.192478	1.055306	0.919841
H	6.793668	2.063553	1.314168
C	6.924146	1.607749	-1.403297
H	6.516202	1.349453	-2.386234
H	6.649789	2.644510	-1.182024
H	8.014457	1.570874	-1.484858
C	6.921439	-0.770785	-0.683070
H	6.645933	-1.505410	0.079699
H	6.490299	-1.099905	-1.634001
H	8.011440	-0.794613	-0.784184
H	-1.187301	4.936029	0.632182
H	-2.887273	5.118691	1.114645
H	-2.290167	4.994769	-1.515337
H	-3.694210	4.083169	-0.917385

L81 – Hexene

Electronic Energy: -1816.75443018
Enthalpy: -1816.014880
Free Energy: -1816.123212

N	-0.575919	1.283536	0.267293
C	0.770717	1.043183	0.276629
N	1.155884	-0.212614	0.317610
H	-0.886177	2.246551	0.320844
C	2.520452	-0.598090	0.146842
C	3.283622	-0.965203	1.269252
C	3.020071	-0.745828	-1.162545
C	4.570871	-1.465404	1.056685
C	4.311407	-1.247183	-1.326247
C	5.084194	-1.607687	-0.226458
H	5.171448	-1.747831	1.918271
H	4.709253	-1.355580	-2.332232
H	6.085817	-2.001120	-0.371152
C	1.640150	2.228637	0.148279
C	2.859005	2.357291	0.829032
C	1.233648	3.272051	-0.698422
C	3.632361	3.496760	0.671718
C	2.023361	4.401593	-0.860988
C	3.233965	4.539980	-0.174661

H	3.192086	1.575390	1.501279
H	0.308064	3.179657	-1.263633
H	4.567233	3.584096	1.219697
H	1.698488	5.191179	-1.533714
C	2.759580	-0.791820	2.662427
H	1.666582	-0.812079	2.700560
H	3.140440	-1.570332	3.328631
H	3.067007	0.168264	3.098090
C	2.185260	-0.374808	-2.351788
H	1.829088	0.661625	-2.304391
H	2.750975	-0.486973	-3.279365
H	1.289145	-1.008588	-2.449437
C	4.077619	5.763975	-0.325760
H	3.696991	6.427471	-1.105220
H	4.114111	6.335908	0.607689
H	5.112656	5.509413	-0.573497
C	-3.995309	0.511527	1.061292
C	-4.200657	0.544057	-0.456016
P	-1.685457	-0.032190	-0.038004
N	-2.838043	0.773251	-0.978256
N	-2.778686	-0.304147	1.208966
C	-2.654146	0.861323	-2.415734
H	-3.103113	0.016701	-2.958075
H	-3.093758	1.787344	-2.799403
H	-1.584454	0.888301	-2.649734
C	-2.301212	-0.639944	2.536096
H	-1.938174	0.229958	3.102124
H	-3.102044	-1.117523	3.107964
H	-1.474421	-1.355785	2.456896
C	-5.196942	1.600548	-0.913157
C	-4.946735	2.966168	-0.291231
C	-4.944786	2.859757	1.227445
C	-3.857617	1.900230	1.691507
H	-5.208615	1.648308	-2.007608
H	-3.977690	3.358593	-0.632114
H	-5.707570	3.674842	-0.632054
H	-4.799485	3.840425	1.691193
H	-5.926695	2.501736	1.567804
H	-2.876314	2.312480	1.416408
H	-3.853335	1.804838	2.782946
H	-6.194684	1.247200	-0.622256
H	-4.556179	-0.448082	-0.785446
H	-4.829715	-0.027885	1.529226
Cr	-0.106190	-1.805403	-0.351059
H	0.421699	-3.346700	-0.562789
H	-1.131305	-1.881516	-2.813390
H	-2.406301	-2.474716	-1.651153
C	-0.529526	-3.571354	-1.562380
C	-1.343258	-2.424281	-1.891768
C	-1.177089	-4.751815	-0.847697
H	-2.080978	-4.390325	-0.335450
H	-1.520772	-5.473355	-1.598399
C	-0.270962	-5.430723	0.175681
H	0.631554	-5.813403	-0.322201
H	-0.783114	-6.304418	0.590924
C	0.131464	-4.479322	1.301446
H	-0.787028	-4.092759	1.771864
H	0.657386	-5.031725	2.091179
C	0.989448	-3.312363	0.825721
H	1.138596	-2.572172	1.619793
H	1.985776	-3.638263	0.501764
H	0.221554	-3.854339	-2.307471

L81 – Octene
Electronic Energy: -1895.36077973
Enthalpy: -1894.559916

Free Energy: -1894.671754

N	-0.292192	1.428722	0.521928
C	1.025984	1.067940	0.398656
N	1.331102	-0.207489	0.398218
H	-0.491747	2.409622	0.679885
C	2.645454	-0.616208	0.022046
C	3.493750	-1.176756	0.995372
C	3.041961	-0.541328	-1.327586
C	4.748952	-1.643303	0.602527
C	4.306658	-1.022121	-1.677408
C	5.158790	-1.566824	-0.724407
H	5.409264	-2.067587	1.355276
H	4.616650	-0.967203	-2.718358
H	6.137403	-1.936236	-1.015628
C	1.970349	2.195307	0.236653
C	3.231565	2.208272	0.849076
C	1.596207	3.298547	-0.544624
C	4.084168	3.287533	0.677923
C	2.464886	4.366448	-0.725915
C	3.723660	4.383586	-0.117904
H	3.538529	1.378357	1.476507
H	0.631557	3.303024	-1.048037
H	5.053038	3.283045	1.170902
H	2.164991	5.202076	-1.353083
C	3.065595	-1.236736	2.426893
H	2.056216	-1.646225	2.526595
H	3.746387	-1.849261	3.022713
H	3.029521	-0.242382	2.890893
C	2.130076	0.021920	-2.372117
H	2.038474	1.113149	-2.300692
H	2.492997	-0.207245	-3.376725
H	1.114011	-0.381188	-2.280615
C	4.660322	5.532691	-0.306781
Cr	-0.335775	-1.801059	0.485427
C	0.989629	-3.514479	0.314062
C	0.745570	-3.134050	-1.149576
C	0.058005	-4.196772	-1.994232
C	-1.319989	-4.613549	-1.499352
C	-2.132252	-2.801339	0.102095
C	-2.281652	-3.448939	-1.265754
H	0.877459	-4.590486	0.431612
H	0.171319	-2.177911	-1.333983
H	0.718215	-5.070185	-2.047140
H	-1.741531	-5.314920	-2.227243
H	-2.952726	-2.088765	0.269166
H	1.988543	-3.209007	0.629003
H	1.715454	-2.847788	-1.573612
H	-0.025846	-3.815069	-3.019868
H	-1.223321	-5.182160	-0.562248
H	-2.236783	-3.571533	0.880215
H	-2.162533	-2.701989	-2.068947
H	-3.311130	-3.818976	-1.378345
C	-0.553982	-2.118032	2.513774
H	-1.623118	-2.142686	2.712581
H	0.016087	-1.379905	3.078838
C	0.078531	-3.342966	2.157768
H	-0.559703	-4.215032	2.048610
H	1.054115	-3.572681	2.577498
H	4.263306	6.268816	-1.009351
H	4.855494	6.048096	0.639609
H	5.632066	5.198093	-0.683250
C	-3.994362	1.204258	0.648153
C	-3.522720	1.583949	-0.743812
P	-1.582539	0.273191	0.364576
N	-2.497166	0.574508	-1.028299

N	-2.750326	0.957774	1.389236
C	-1.836210	0.589377	-2.317381
H	-2.570984	0.474640	-3.118610
H	-1.260607	1.511054	-2.502024
H	-1.146074	-0.259538	-2.383391
C	-2.868451	0.510921	2.766901
H	-3.353533	1.288858	3.363204
H	-3.453389	-0.415587	2.869246
H	-1.875489	0.346320	3.192273
C	-4.694946	1.648991	-1.702983
C	-5.683611	2.690699	-1.174148
C	-6.103184	2.423316	0.270280
C	-4.906980	2.276267	1.213785
H	-4.365763	1.915464	-2.713108
H	-5.216409	3.683310	-1.236859
H	-6.565287	2.728615	-1.820702
H	-6.761012	3.222688	0.624538
H	-6.695657	1.499028	0.308654
H	-4.353937	3.221944	1.296702
H	-5.247767	2.013244	2.220848
H	-5.165043	0.658498	-1.767132
H	-3.060751	2.591981	-0.689492
H	-4.574822	0.264824	0.564739

L82 – Hexene
Electronic Energy: -1701.66666114
Enthalpy: -1701.025253
Free Energy: -1701.127118

N	0.489380	1.871292	0.692901
C	1.186655	0.709081	0.474143
N	0.486958	-0.389336	0.309389
H	1.010306	2.703489	0.942573
C	1.102791	-1.592099	-0.164928
C	1.359554	-2.654011	0.718281
C	1.309853	-1.725914	-1.553376
C	1.843608	-3.852449	0.185327
C	1.790048	-2.941251	-2.040019
C	2.055666	-4.001525	-1.178696
H	2.052424	-4.677821	0.862121
H	1.955153	-3.050317	-3.109137
H	2.426591	-4.942819	-1.572744
C	2.649600	0.847413	0.363087
C	3.540607	-0.098227	0.890357
C	3.173818	1.958633	-0.316268
C	4.907828	0.067329	0.736290
C	4.543979	2.103185	-0.481961
C	5.437457	1.161507	0.038692
H	3.164299	-0.948323	1.447885
H	2.502226	2.694169	-0.752941
H	5.584871	-0.667276	1.164763
H	4.929474	2.960049	-1.028345
C	1.163388	-2.525922	2.199357
H	0.609186	-1.623841	2.472607
H	0.626064	-3.389421	2.603146
H	2.122891	-2.487938	2.730033
C	1.027887	-0.586963	-2.485158
H	1.705614	0.259437	-2.317454
H	1.140846	-0.893237	-3.527323
H	0.008955	-0.186453	-2.373667
C	6.912391	1.303488	-0.151690
H	7.180162	2.288612	-0.539671
H	7.456148	1.146713	0.784422
H	7.290443	0.557747	-0.859757
P	-1.195965	1.900437	0.405791
O	-1.220578	3.270497	-0.450593

O	-1.910110	2.400809	1.782040
C	-2.499764	3.935923	-0.657127
H	-2.687500	4.568583	0.215733
H	-3.301706	3.187861	-0.704212
C	-2.411790	4.729655	-1.927065
H	-3.344824	5.275462	-2.087689
H	-1.598755	5.458262	-1.878752
H	-2.242911	4.080905	-2.790261
C	-2.662114	1.432716	2.556624
H	-3.160939	2.029615	3.322320
H	-3.444937	0.996862	1.917237
C	-1.785654	0.368242	3.163204
H	-0.973798	0.811480	3.746472
H	-2.372346	-0.274283	3.825515
H	-1.339158	-0.274340	2.392061
Cr	-1.588660	-0.372345	-0.281746
H	-2.333627	-1.739352	-0.804172
H	-2.474337	0.902793	-2.435433
H	-3.771447	1.027431	-1.159241
C	-3.190277	-1.007789	-1.624249
C	-2.976669	0.420519	-1.595548
C	-4.468294	-1.562299	-1.003618
H	-4.867827	-0.807232	-0.310513
H	-5.219889	-1.676603	-1.793381
C	-4.283063	-2.872478	-0.244148
H	-3.926999	-3.654996	-0.928969
H	-5.253322	-3.213401	0.129999
C	-3.298792	-2.725620	0.914687
H	-3.653506	-1.918412	1.576576
H	-3.306560	-3.633692	1.531715
C	-1.877468	-2.426230	0.456793
H	-1.217292	-2.203757	1.301502
H	-1.432176	-3.268836	-0.086255
H	-2.870830	-1.521016	-2.537300

L82 – Octene
Electronic Energy: -1780.27427620
Enthalpy: -1779.572058
Free Energy: -1779.677594

N	0.470131	-1.976559	0.011003
C	1.223431	-0.836346	-0.150920
N	0.604337	0.301768	-0.340245
H	0.958350	-2.864165	-0.020508
C	1.352078	1.521815	-0.343441
C	1.529483	2.204690	-1.561618
C	1.822537	2.068487	0.867248
C	2.190232	3.434636	-1.552721
C	2.484940	3.298076	0.827467
C	2.671693	3.980245	-0.368862
H	2.330654	3.959852	-2.494571
H	2.853958	3.720628	1.759041
H	3.185990	4.936417	-0.377247
C	2.682376	-1.045801	-0.036823
C	3.598732	-0.406453	-0.883649
C	3.172375	-1.919684	0.944949
C	4.958329	-0.633892	-0.742496
C	4.538034	-2.123511	1.091706
C	5.456749	-1.486525	0.252144
H	3.245240	0.253870	-1.667625
H	2.480766	-2.414468	1.623422
H	5.653171	-0.140053	-1.417127
H	4.900330	-2.787463	1.872254
C	1.055108	1.606241	-2.848378
H	0.110772	1.072317	-2.719477
H	0.925995	2.368065	-3.621445

H	1.766582	0.869146	-3.244116
C	1.598213	1.382301	2.177548
H	2.032265	0.376522	2.210665
H	2.038935	1.954362	2.996826
H	0.529143	1.270547	2.396557
C	6.927122	-1.705908	0.402546
Cr	-1.701644	0.424855	-0.304550
C	-1.801166	2.542027	-0.770585
C	-1.628256	2.551250	0.751843
C	-2.783532	3.167709	1.526737
C	-4.129949	2.493675	1.305069
C	-3.676180	0.179109	0.325515
C	-4.117017	0.984136	1.539944
H	-2.600050	3.226594	-1.047716
H	-1.417318	1.555543	1.242910
H	-2.846495	4.228350	1.257275
H	-4.861080	2.973535	1.963921
H	-3.843241	-0.893221	0.504285
H	-0.874372	2.833868	-1.264830
H	-0.682330	3.063966	0.964537
H	-2.535015	3.138247	2.595340
H	-4.481762	2.688313	0.281002
H	-4.315317	0.437156	-0.531777
H	-3.483220	0.757510	2.414771
H	-5.127933	0.665951	1.833837
C	-2.214091	-0.070231	-2.247295
H	-3.059116	-0.752749	-2.184617
H	-1.349766	-0.451733	-2.791947
C	-2.499799	1.322420	-2.283179
H	-3.540504	1.617680	-2.186889
H	-1.927894	1.957013	-2.954129
H	7.154529	-2.382305	1.229161
H	7.361584	-2.131885	-0.507738
H	7.453696	-0.763609	0.585370
P	-1.234366	-1.927996	0.085828
O	-1.637818	-2.791007	1.407244
O	-1.535527	-3.032577	-1.055859
C	-2.048769	-2.104372	2.616777
H	-2.269318	-2.909520	3.320373
H	-2.984651	-1.566956	2.420804
C	-0.987151	-1.179264	3.147331
H	-1.314581	-0.720115	4.084132
H	-0.047483	-1.707257	3.334547
H	-0.783526	-0.367658	2.436493
C	-2.907451	-3.497188	-1.197259
H	-3.106486	-4.215176	-0.394965
H	-3.596255	-2.649653	-1.065601
C	-3.044549	-4.116344	-2.557120
H	-2.344881	-4.946823	-2.678676
H	-4.057124	-4.505918	-2.687539
H	-2.852927	-3.386897	-3.348457

L83 – Hexene

Electronic Energy: -1046.17168431
Enthalpy: -1045.811337
Free Energy: -1045.878433

N	0.305930	-2.038913	-0.211415
C	1.327964	-1.202332	-0.421287
C	3.734894	-0.962456	0.187156
C	3.711883	0.343923	-0.593599
C	2.498548	1.239497	-0.325653
C	0.844522	-3.151989	0.380630
C	2.191641	-2.962164	0.558335
N	2.484314	-1.716246	0.051745
H	2.622142	2.212991	-0.807685

H	2.372753	1.432813	0.744952
H	4.623147	0.889428	-0.330372
H	3.789906	0.130044	-1.665639
H	4.558287	-1.595116	-0.153237
H	3.884572	-0.773004	1.255864
H	0.243802	-4.009270	0.645852
H	2.955200	-3.590882	0.990345
P	0.949619	0.461710	-0.968749
C	1.173998	0.473549	-2.784150
H	0.857568	1.448034	-3.166305
H	2.205853	0.290329	-3.094544
H	0.530020	-0.283556	-3.237774
Cr	-1.390355	-0.683348	-0.327148
H	-4.110759	-0.554056	-1.253956
H	-2.933132	-1.096342	0.012514
H	-2.099474	1.737113	-1.204570
H	-2.289022	0.490505	-2.532405
C	-3.398502	0.064026	-0.698334
C	-2.375786	0.716405	-1.468609
C	-2.460697	-1.834045	1.195869
C	-3.989681	0.777177	0.510300
C	-4.286781	-0.139356	1.694915
C	-3.035899	-0.850241	2.208135
H	-3.164452	-2.646961	0.980070
H	-1.532866	-2.299458	1.544460
H	-3.281056	1.554114	0.833213
H	-4.898479	1.307351	0.200858
H	-4.738135	0.447837	2.500431
H	-5.037217	-0.889156	1.407251
H	-2.275355	-0.091707	2.460042
H	-3.253863	-1.369990	3.150133

L83 – Octene
Electronic Energy: -1124.78323387
Enthalpy: -1124.361300
Free Energy: -1124.432480

N	0.385877	-2.094988	0.518228
C	1.406274	-1.240047	0.397274
C	2.499477	1.148275	-0.324025
C	3.761111	0.297106	-0.160204
C	3.651357	-1.115446	-0.711809
C	0.830276	-3.278765	-0.007684
C	2.111623	-3.124738	-0.475502
N	2.463729	-1.821030	-0.221040
H	4.535456	-1.699466	-0.443896
H	3.588361	-1.098297	-1.805758
H	4.590258	0.781892	-0.684085
H	4.056060	0.256834	0.894240
H	2.692203	2.185806	-0.037583
H	2.166370	1.167428	-1.367164
Cr	-1.310558	-0.501929	0.569830
C	-2.801465	-2.080718	0.368073
C	-2.568210	-1.684728	-1.094586
C	-3.789497	-1.100691	-1.789108
C	-4.334729	0.167962	-1.147571
C	-2.467318	1.170776	0.272032
C	-3.291591	1.274692	-0.998521
H	-3.868224	-2.225999	0.527501
H	-1.713032	-0.978792	-1.289714
H	-4.567325	-1.873059	-1.814015
H	-5.178478	0.517499	-1.751288
H	-1.726672	1.981889	0.328546
H	-2.260815	-2.992560	0.625005
H	-2.202986	-2.576441	-1.617081
H	-3.529002	-0.893730	-2.834352

H	-4.754006	-0.064232	-0.156971
H	-3.121114	1.276910	1.149796
H	-2.640563	1.281620	-1.887005
H	-3.802839	2.247981	-1.015791
C	-1.590745	-0.509737	2.597598
H	-1.687743	0.537183	2.881621
H	-0.810234	-1.073116	3.107825
C	-2.765665	-1.219683	2.209197
H	-3.693169	-0.657286	2.133966
H	-2.900011	-2.226672	2.592997
H	0.214261	-4.166531	-0.022838
H	2.792115	-3.810609	-0.956890
P	1.120896	0.505736	0.724279
C	1.695487	0.838036	2.427908
H	1.478092	1.882353	2.668791
H	1.145853	0.212650	3.133837
H	2.765447	0.661898	2.562894

L84 – Hexene
Electronic Energy: -1008.07057319
Enthalpy: -1007.718705
Free Energy: -1007.787541

N	0.387952	-1.664082	0.621102
C	1.353173	-0.813686	0.241374
C	3.791102	-0.894145	-0.323802
C	1.027807	1.527290	-1.496170
C	0.952434	-2.906381	0.670562
C	2.274760	-2.806069	0.314591
N	2.515815	-1.481731	0.044005
H	0.593669	0.860697	-2.244162
H	0.528034	2.496039	-1.585678
H	4.338241	-1.580983	-0.969040
H	4.388751	-0.683071	0.566084
H	0.389793	-3.785785	0.946237
H	3.053446	-3.548275	0.223758
P	0.733844	0.877772	0.180818
C	1.828555	1.891670	1.229718
H	1.459408	2.920523	1.231561
H	1.816896	1.529028	2.259291
H	2.858395	1.900061	0.862563
Cr	-1.364717	-0.420618	0.804025
H	-4.087334	-0.511949	-0.062291
H	-2.840866	-0.999100	1.184454
H	-2.363934	1.991098	0.167075
H	-2.430771	0.849907	-1.260218
C	-3.448276	0.140355	0.541008
C	-2.520049	0.969310	-0.179499
C	-2.233975	-1.730361	2.317292
C	-4.115206	0.690255	1.795252
C	-4.261485	-0.325006	2.926278
C	-2.914115	-0.880293	3.384421
H	-2.814909	-2.632516	2.090645
H	-1.234439	-2.061487	2.622173
H	-3.519353	1.540083	2.159072
H	-5.094530	1.102029	1.523310
H	-4.776974	0.145883	3.768843
H	-4.903987	-1.155740	2.601446
H	-2.258811	-0.037104	3.660003
H	-3.038156	-1.466092	4.304462
H	2.090618	1.671021	-1.710004
H	3.614282	0.032480	-0.871559

L84 – Octene
Electronic Energy: -1086.68041492
Enthalpy: -1086.267292

Free Energy: -1086.341298

N	0.365582	-1.912445	0.093040
C	1.387904	-1.058237	0.239486
C	3.895335	-1.159596	0.381861
C	1.598499	1.656003	-0.844352
C	0.914823	-3.153402	-0.048745
C	2.282729	-3.053323	0.017786
N	2.571455	-1.725071	0.199800
H	1.211639	2.675809	-0.768874
H	2.688527	1.700012	-0.771276
H	4.600052	-1.646415	-0.292272
H	4.232312	-1.293282	1.412576
Cr	-1.425386	-0.524541	0.464281
C	-2.827294	-2.120315	0.083564
C	-2.734815	-1.456194	-1.296405
C	-4.032904	-0.830636	-1.785569
C	-4.590183	0.264766	-0.886130
C	-2.689639	1.101126	0.592181
C	-3.595639	1.388153	-0.592570
H	-3.868872	-2.356154	0.292932
H	-1.929112	-0.678507	-1.420090
H	-4.772692	-1.631238	-1.902379
H	-5.490652	0.666517	-1.362437
H	-2.015976	1.948751	0.786508
H	-2.231187	-3.033203	0.120082
H	-2.369462	-2.215940	-1.996696
H	-3.863696	-0.421996	-2.789481
H	-4.927986	-0.169986	0.066889
H	-3.298647	0.971973	1.499027
H	-3.001903	1.594527	-1.497767
H	-4.154910	2.316120	-0.404199
C	-1.514667	-0.896012	2.480011
H	-1.662527	0.071735	2.956337
H	-0.651150	-1.467556	2.818746
C	-2.665701	-1.622334	2.056799
H	-3.633122	-1.138587	2.163474
H	-2.692567	-2.691943	2.242951
H	0.313449	-4.038778	-0.195023
H	3.065149	-3.794201	-0.050345
P	0.844019	0.647741	0.475162
C	1.620741	1.270794	2.001106
H	1.213613	2.262020	2.218588
H	1.377099	0.619901	2.843693
H	2.707183	1.359261	1.915713
H	3.869755	-0.095230	0.147946
H	1.320434	1.263801	-1.824810

L85 – Hexene
Electronic Energy: -1386.16158622
Enthalpy: -1385.933445
Free Energy: -1386.001323

N	0.470969	-1.563827	0.682957
C	1.452019	-0.780202	0.169319
C	0.945940	-2.814032	0.779219
C	2.250170	-2.859872	0.330353
N	2.519928	-1.575892	-0.041934
P	0.804412	0.881398	0.059818
Cr	-1.327940	-0.309459	0.900404
H	-3.984387	-0.481184	-0.090693
H	-2.790374	-0.924092	1.226917
H	-2.372864	2.077757	0.350613
H	-2.355881	1.019506	-1.144960
C	-3.424270	0.186608	0.571308
C	-2.499845	1.077908	-0.066060

C	-2.182426	-1.658264	2.358848
C	-4.186449	0.644102	1.806263
C	-4.355665	-0.434943	2.872322
C	-3.012540	-0.927682	3.405993
H	-2.637599	-2.608977	2.057828
H	-1.171658	-1.883679	2.721213
H	-3.656223	1.501395	2.244687
H	-5.163597	1.022988	1.485454
H	-4.957065	-0.037858	3.694873
H	-4.922071	-1.282061	2.460703
H	-2.446797	-0.065199	3.791343
H	-3.164785	-1.586622	4.269971
F	0.227714	-3.810601	1.238108
F	3.126213	-3.812344	0.223880
F	1.879253	1.804916	0.774489
F	1.073855	1.347285	-1.432749
F	3.704930	-1.193580	-0.545426

L85 – Octene
Electronic Energy: -1464.77662286
Enthalpy: -1464.487135
Free Energy: -1464.560918

N	0.462493	-1.897219	-0.023291
C	1.475025	-1.068121	0.305144
C	0.988289	-3.097270	-0.292040
C	2.359133	-3.068425	-0.139273
N	2.617702	-1.783911	0.238130
Cr	-1.478762	-0.473549	0.409670
C	-2.837385	-2.102346	0.144954
C	-2.805314	-1.496403	-1.266177
C	-4.128677	-0.913402	-1.737038
C	-4.661965	0.223216	-0.875145
C	-2.713812	1.145300	0.487948
C	-3.658275	1.358479	-0.677217
H	-3.861785	-2.372650	0.391294
H	-2.014390	-0.715184	-1.455833
H	-4.861514	-1.727066	-1.781772
H	-5.576477	0.602066	-1.341588
H	-1.991756	1.970712	0.577811
H	-2.198109	-2.984985	0.209036
H	-2.450273	-2.286357	-1.938058
H	-4.001151	-0.558185	-2.766451
H	-4.968324	-0.162343	0.108784
H	-3.270680	1.090253	1.433074
H	-3.097296	1.521657	-1.610158
H	-4.206308	2.296400	-0.509322
C	-1.482581	-0.776689	2.436958
H	-1.602657	0.210863	2.880265
H	-0.622683	-1.345743	2.790200
C	-2.656889	-1.503867	2.080222
H	-3.614156	-0.999298	2.183452
H	-2.693025	-2.561323	2.322960
P	0.861096	0.562337	0.690760
F	1.814817	1.546140	-0.116152
F	1.414230	0.871195	2.148404
F	3.858547	-1.326057	0.489170
F	3.301902	-3.952781	-0.284162
F	0.247530	-4.123591	-0.650298

L86 – Hexene
Electronic Energy: -2186.37912596
Enthalpy: -2186.118466
Free Energy: -2186.200280

C	1.371570	-1.364074	-0.916898

C	3.733470	-1.027072	0.269123
C	3.649376	0.425335	-0.261605
C	2.273579	1.130745	-0.194971
C	0.799207	-3.211982	0.204191
C	2.133678	-3.478491	0.093226
P	0.883760	0.340185	-1.198237
Cr	-1.356221	-0.712201	-0.344791
H	-4.070971	-0.948388	-1.130618
H	-2.822169	-1.114816	0.221840
H	-2.298638	1.525711	-1.444401
H	-2.397752	0.102008	-2.596470
C	-3.444100	-0.164364	-0.695348
C	-2.501883	0.462518	-1.572225
C	-2.173428	-1.516105	1.483884
C	-4.108687	0.662267	0.395893
C	-4.220128	-0.034845	1.748859
C	-2.852731	-0.427092	2.301659
H	-2.718628	-2.465998	1.520261
H	-1.152695	-1.715410	1.833393
H	-3.535601	1.591390	0.521279
H	-5.100245	0.962910	0.038568
H	-4.728650	0.629588	2.452965
H	-4.851028	-0.930179	1.662131
H	-2.209977	0.467214	2.335791
H	-2.941355	-0.761681	3.342695
P	2.940341	-2.266600	-0.977963
N	0.384570	-2.010993	-0.311402
F	1.390820	0.718795	-2.668994
F	1.858711	1.158791	1.094529
F	2.460402	2.391843	-0.630232
F	4.521630	1.169026	0.432738
F	4.017840	0.391899	-1.569915
F	3.154265	-1.094536	1.485064
F	5.032296	-1.339340	0.399744
F	2.683124	-4.601390	0.507273
F	-0.094017	-3.980307	0.787571

L86 – Octene (msr-17a-pcn04F-oct2-fr-TS)
Electronic Energy: -2264.99515203
Enthalpy: -2264.673188
Free Energy: -2264.758997

C	1.446125	-1.344197	0.351187
C	3.290454	-1.480998	2.377265
C	3.271980	0.047314	2.339195
C	1.895687	0.690126	2.177734
C	0.749723	-3.468636	0.337881
C	2.019008	-3.721925	0.757920
H	1.967057	1.775130	2.309962
H	1.214010	0.332702	2.957843
H	3.682976	0.392951	3.294719
H	3.965292	0.419527	1.574826
H	4.267156	-1.840476	2.708608
H	2.539362	-1.869834	3.072502
Cr	-1.308994	-0.576542	0.414283
C	-2.785784	-2.100825	-0.013131
C	-2.611068	-1.431071	-1.383709
C	-3.858111	-0.744123	-1.920704
C	-4.399612	0.372176	-1.037840
C	-2.526060	1.074636	0.540123
C	-3.360461	1.433256	-0.676285
H	-3.846671	-2.262516	0.168362
H	-1.769680	-0.686934	-1.471520
H	-4.628417	-1.509038	-2.072751
H	-5.248775	0.830207	-1.555435
H	-1.816633	1.877851	0.787024

H	-2.259682	-3.055451	0.017552
H	-2.251903	-2.201478	-2.074917
H	-3.627080	-0.340492	-2.914170
H	-4.811748	-0.052239	-0.110042
H	-3.179355	0.945551	1.415072
H	-2.716931	1.627716	-1.549389
H	-3.877712	2.385522	-0.489960
C	-1.446085	-0.983172	2.417947
H	-1.575100	-0.022919	2.914584
H	-0.611473	-1.591051	2.769033
C	-2.615734	-1.663071	1.962700
H	-3.566635	-1.149578	2.076147
H	-2.680470	-2.734330	2.130294
H	-0.011352	-4.218211	0.144198
H	2.420467	-4.718438	0.896586
P	1.050570	0.407360	0.555006
C	2.091347	1.306625	-0.643040
H	1.950279	2.382224	-0.510476
H	3.152224	1.071802	-0.519075
H	1.794912	1.051081	-1.662365
P	2.975995	-2.216066	0.677490
N	0.404558	-2.128444	0.158904

L87 – Hexene

Electronic Energy: -1584.66727556
Enthalpy: -1584.144104
Free Energy: -1584.228242

C	1.795868	-1.366866	-0.318770
N	2.009111	-0.034004	-0.076746
P	0.571929	0.957705	-0.150094
C	0.547947	1.719558	1.534976
C	0.967598	2.292434	-1.363994
C	4.126041	-1.975638	0.279540
Cr	-1.490828	-0.374851	-0.531044
H	-3.825485	0.195582	-2.041560
H	-3.092291	-0.711126	-0.637632
H	-2.149494	2.298189	-0.635287
H	-1.827205	1.579758	-2.281175
C	-3.373865	0.569254	-1.116743
C	-2.218200	1.418169	-1.275331
C	-2.919683	-1.823279	0.349580
C	-4.378163	0.884316	-0.015987
C	-4.990322	-0.353382	0.634023
C	-3.933043	-1.219304	1.315132
H	-3.369379	-2.583508	-0.299093
H	-2.092903	-2.302616	0.884506
H	-3.869459	1.477763	0.758868
H	-5.161109	1.530774	-0.429558
H	-5.744749	-0.045132	1.364305
H	-5.521670	-0.946530	-0.123705
H	-3.407958	-0.603824	2.062786
H	-4.415136	-2.024118	1.885059
C	4.396825	-0.502100	0.046651
C	3.260537	0.338456	0.599243
C	1.007369	-3.686588	-0.724803
C	2.315508	-3.595883	-0.376407
N	2.758590	-2.297243	-0.141090
H	4.235894	-2.235336	1.338924
H	4.812654	-2.606056	-0.290694
H	5.335336	-0.225002	0.531491
H	4.507881	-0.301242	-1.024898
H	3.443928	1.401925	0.440243
H	3.159539	0.181506	1.684840
H	3.042070	-4.393400	-0.285348
H	0.514361	-4.616838	-0.970628

H	1.548095	2.142065	1.708169
H	0.035194	2.874837	-1.378734
C	2.114200	3.225647	-0.997006
H	3.085692	2.736031	-1.118344
H	2.114561	4.088886	-1.669437
H	2.045907	3.612641	0.024533
C	1.171547	1.666690	-2.739478
H	2.086558	1.064459	-2.763811
H	0.339254	1.017414	-3.031239
H	1.268963	2.445915	-3.500918
C	-0.479158	2.840568	1.628301
H	-0.410384	3.327772	2.605344
H	-0.339433	3.614608	0.866954
H	-1.499705	2.451580	1.533473
C	0.277074	0.626774	2.563123
H	-0.719503	0.187248	2.415715
H	1.003903	-0.190378	2.516615
H	0.302670	1.036116	3.577297
P	0.278392	-2.075801	-0.847963

L87 – Octene
Electronic Energy: -1663.27533276
Enthalpy: -1662.690258
Free Energy: -1662.779608

C	1.862378	-1.384574	-0.165316
N	2.091201	-0.025167	-0.170087
P	0.740641	1.011491	0.148978
C	1.381328	2.150668	1.453572
C	0.531273	2.049503	-1.377358
C	4.101603	-1.851462	-1.156813
C	4.126942	-0.366972	-1.462870
C	3.485715	0.412606	-0.328628
C	1.123626	-3.748170	-0.094373
C	2.362408	-3.573521	-0.623541
N	2.776290	-2.249877	-0.670176
H	3.500330	1.484467	-0.528191
H	4.032493	0.245526	0.611542
H	5.161765	-0.046977	-1.604913
H	3.588072	-0.161197	-2.394615
H	4.329391	-2.448289	-2.043151
H	4.839866	-2.103837	-0.386846
Cr	-1.400205	-0.322471	0.589521
C	-3.009554	-1.808136	0.504965
C	-2.784966	-1.505558	-0.980694
C	-3.977455	-0.883475	-1.691430
C	-4.448374	0.438461	-1.102121
C	-2.532920	1.392383	0.293156
C	-3.351281	1.495563	-0.984207
H	-4.079052	-1.818566	0.706642
H	-1.891833	-0.867352	-1.229471
H	-4.798590	-1.609875	-1.683083
H	-5.268706	0.812982	-1.723070
H	-1.858243	2.253962	0.386302
H	-2.579557	-2.771978	0.775618
H	-2.477549	-2.441178	-1.460979
H	-3.711069	-0.734807	-2.745701
H	-4.884538	0.270348	-0.105867
H	-3.206032	1.447226	1.161643
H	-2.702383	1.452457	-1.874765
H	-3.818893	2.490179	-1.024863
C	-1.600289	-0.208500	2.632395
H	-1.684004	0.850166	2.874378
H	-0.792963	-0.748064	3.124881
C	-2.797764	-0.921656	2.335302
H	-3.722998	-0.352399	2.305388

H	-2.913902	-1.919420	2.747879
H	0.652456	-4.714951	0.019182
H	3.048675	-4.324552	-0.994396
C	1.647053	3.034606	-1.702433
H	2.543748	2.525471	-2.069658
H	1.320321	3.707577	-2.501293
H	1.930971	3.661500	-0.851949
H	-0.377104	2.623860	-1.141674
C	0.226947	1.143102	-2.563813
H	-0.612925	0.467251	-2.366780
H	-0.032243	1.738237	-3.444371
H	1.092464	0.524406	-2.825307
C	0.367892	3.251817	1.743079
H	-0.553803	2.839556	2.168394
H	0.777894	3.954062	2.474905
H	0.099165	3.828890	0.852056
H	2.292825	2.610700	1.045853
C	1.743285	1.369784	2.710026
H	0.856274	0.918118	3.165233
H	2.461166	0.568032	2.513531
H	2.188798	2.038582	3.452396
P	0.445254	-2.208108	0.458426

L88 – Hexene

Electronic Energy: -1427.42376205
Enthalpy: -1427.019777
Free Energy: -1427.092570

C	1.711007	-1.384951	-0.382057
N	1.905412	-0.042820	-0.207771
P	0.454297	0.904249	-0.384894
C	3.923174	-1.936067	0.553803
Cr	-1.560661	-0.452036	-0.808714
H	-4.103220	0.481365	-1.866673
H	-3.182854	-0.722783	-0.947112
H	-2.057122	2.258611	-0.562878
H	-2.021325	1.705999	-2.301676
C	-3.431022	0.641830	-1.017529
C	-2.263151	1.452122	-1.268268
C	-3.010348	-2.035388	-0.227764
C	-4.130836	0.803115	0.326837
C	-4.680496	-0.496413	0.906680
C	-3.592800	-1.551103	1.093311
H	-3.789611	-2.447690	-0.879902
H	-2.266409	-2.821703	-0.090266
H	-3.406740	1.225510	1.041361
H	-4.928483	1.549191	0.227230
H	-5.168749	-0.285153	1.863057
H	-5.462058	-0.898519	0.247088
H	-2.789829	-1.127664	1.723683
H	-3.984892	-2.404537	1.661828
C	4.282674	-0.534649	0.098130
C	3.155478	0.439542	0.392552
C	0.928731	-3.716443	-0.699683
C	2.186360	-3.614658	-0.200328
N	2.625477	-2.305332	-0.016885
H	3.861941	-1.997642	1.646788
H	4.661406	-2.667397	0.217740
H	5.189582	-0.204900	0.609318
H	4.496080	-0.539600	-0.975780
H	3.383098	1.427274	-0.019896
H	3.023105	0.557104	1.478041
H	2.877374	-4.410941	0.045582
H	0.450589	-4.658966	-0.928377
P	0.264260	-2.111086	-1.067486
C	0.324810	1.744483	1.225519

H	1.230308	2.307658	1.469504
H	-0.511406	2.448549	1.200016
H	0.132110	1.016002	2.017639
C	0.957749	2.233741	-1.513406
H	0.173902	2.994387	-1.552304
H	1.881458	2.715934	-1.180908
H	1.104020	1.836734	-2.520115

L88 – Octene

Electronic Energy: -1506.03354831
Enthalpy: -1505.568173
Free Energy: -1505.646711

C	1.890665	-1.475686	-0.331201
N	2.061333	-0.109177	-0.310664
P	0.647820	0.859085	-0.099966
C	3.389394	0.440785	-0.605939
C	4.451489	-0.430536	0.038566
C	4.343025	-1.853225	-0.470544
C	1.262877	-3.873084	-0.272417
C	2.601262	-3.654908	-0.340335
N	2.954789	-2.312936	-0.369834
H	4.966839	-2.536431	0.110004
H	4.658733	-1.921010	-1.518293
H	5.444857	-0.037532	-0.188094
H	4.327156	-0.409226	1.126503
H	3.434607	1.460943	-0.216548
H	3.537893	0.495388	-1.694175
Cr	-1.424221	-0.465477	0.317010
C	-3.101529	-1.847317	0.398027
C	-3.104282	-1.444789	-1.082240
C	-4.353087	-0.707793	-1.540987
C	-4.602447	0.613128	-0.826799
C	-2.425031	1.362098	0.278920
C	-3.413237	1.573682	-0.857236
H	-4.123682	-1.843739	0.771259
H	-2.227405	-0.832838	-1.435355
H	-5.214244	-1.373173	-1.410189
H	-5.479486	1.084479	-1.281681
H	-1.690725	2.180662	0.298512
H	-2.668571	-2.838780	0.533990
H	-2.939721	-2.356880	-1.666620
H	-4.267904	-0.525521	-2.619337
H	-4.877870	0.425426	0.221837
H	-2.955638	1.415326	1.240904
H	-2.909310	1.506191	-1.835740
H	-3.793292	2.604293	-0.806285
C	-1.297261	-0.449531	2.366134
H	-1.280127	0.596565	2.667053
H	-0.455884	-1.054735	2.700733
C	-2.567298	-1.079761	2.220944
H	-3.450017	-0.460941	2.361006
H	-2.683092	-2.092674	2.594387
H	0.816319	-4.857242	-0.242036
H	3.400817	-4.383901	-0.378964
P	0.366246	-2.345382	-0.295415
H	1.344222	1.407256	2.147842
H	0.259300	2.639702	1.480972
H	1.555715	2.491139	-1.685993
H	0.439619	1.340973	-2.462566
H	-0.193182	2.662377	-1.466164
H	1.959344	2.618929	0.996780
C	0.620190	1.937362	-1.564556
C	1.105107	1.985128	1.251951

L89 – Hexene

Electronic Energy: -1506.04860719
Enthalpy: -1505.584199
Free Energy: -1505.663520

C	1.778996	-1.367057	-0.423449
N	2.020474	-0.034753	-0.232418
P	0.604280	0.972783	-0.375018
C	3.946068	-1.991097	0.556882
Cr	-1.450636	-0.373754	-0.617487
H	-3.927331	0.443115	-1.752559
H	-3.058887	-0.688247	-0.624883
H	-2.075969	2.271030	-0.199872
H	-1.976697	1.872141	-1.978866
C	-3.368959	0.645625	-0.832617
C	-2.228952	1.520420	-0.977773
C	-2.812552	-1.981057	0.114996
C	-4.245428	0.756543	0.407741
C	-4.823354	-0.579960	0.864560
C	-3.733686	-1.573441	1.262431
H	-3.334283	-2.590688	-0.632067
H	-1.968010	-2.572622	0.480125
H	-3.647110	1.189644	1.223391
H	-5.048194	1.475333	0.205650
H	-5.500306	-0.415238	1.708313
H	-5.437023	-1.009221	0.059760
H	-3.135984	-1.130304	2.073651
H	-4.190594	-2.472867	1.695256
C	4.382993	-0.635737	0.034585
C	3.316821	0.413969	0.293099
C	0.907066	-3.666546	-0.732080
C	2.156965	-3.613507	-0.208142
N	2.645367	-2.321117	-0.028503
H	3.857394	-1.988447	1.650075
H	4.652478	-2.776148	0.279515
H	5.312622	-0.334233	0.521722
H	4.584896	-0.705429	-1.039759
H	3.583278	1.358605	-0.193010
H	3.229371	0.611536	1.371497
H	2.810233	-4.434428	0.060047
H	0.395263	-4.591222	-0.961831
P	0.323539	-2.040399	-1.155155
C	0.487109	1.763481	1.272669
H	1.459105	2.177880	1.564883
H	-0.188710	2.618926	1.156422
C	1.140275	2.299760	-1.509833
H	0.312942	3.017517	-1.555816
H	1.981459	2.837643	-1.055025
C	1.494575	1.775465	-2.891301
H	2.330275	1.069421	-2.851928
H	0.650815	1.255072	-3.355982
H	1.783488	2.594453	-3.553731
C	-0.044983	0.781030	2.303059
H	-1.003285	0.350831	1.974314
H	0.642825	-0.056192	2.460702
H	-0.213494	1.260682	3.269959

L89 – Octene
Electronic Energy: -1584.65697996
Enthalpy: -1584.130474
Free Energy: -1584.211739

C	1.871640	-1.466068	-0.272618
N	1.993276	-0.105847	-0.448463
P	0.614702	0.858356	-0.038511
C	4.284406	-1.810486	-0.697385
C	4.178141	-0.515817	-1.476265

C	3.309739	0.481124	-0.732097
C	1.322732	-3.850804	0.128382
C	2.630277	-3.627084	-0.161226
N	2.938073	-2.292207	-0.385280
H	3.164488	1.384816	-1.332404
H	3.794009	0.785991	0.208015
H	5.173333	-0.092413	-1.627268
H	3.750509	-0.713995	-2.465146
H	4.794779	-2.586764	-1.271621
H	4.837842	-1.665666	0.238366
Cr	-1.418418	-0.480225	0.568458
C	-3.101294	-1.848217	0.364314
C	-2.893228	-1.387976	-1.085050
C	-4.046794	-0.599385	-1.687243
C	-4.404054	0.683846	-0.950766
C	-2.414387	1.346181	0.498345
C	-3.229591	1.641886	-0.749822
H	-4.167712	-1.854040	0.583003
H	-1.951600	-0.804913	-1.291871
H	-4.922982	-1.256552	-1.734516
H	-5.204514	1.180766	-1.508474
H	-1.691239	2.152400	0.693551
H	-2.695823	-2.849028	0.516043
H	-2.675992	-2.285949	-1.674717
H	-3.790656	-0.359341	-2.727140
H	-4.835092	0.442103	0.032450
H	-3.081552	1.336146	1.372487
H	-2.594036	1.636440	-1.651156
H	-3.620260	2.668037	-0.686205
C	-1.583029	-0.557225	2.606008
H	-1.595523	0.473012	2.959079
H	-0.811796	-1.196730	3.032407
C	-2.830105	-1.158505	2.252068
H	-3.714802	-0.528240	2.294101
H	-3.012430	-2.178852	2.575952
H	0.909537	-4.831415	0.319975
H	3.435326	-4.346246	-0.244122
P	0.396996	-2.340466	0.102548
C	0.389484	1.938471	-1.499286
H	-0.449611	2.601975	-1.255334
H	1.265360	2.588331	-1.611611
C	1.260581	1.978851	1.259194
H	2.038841	2.613313	0.816460
H	0.436567	2.650510	1.530344
C	0.115821	1.154270	-2.770710
H	0.963561	0.518472	-3.044514
H	-0.758148	0.500950	-2.663819
H	-0.080847	1.826714	-3.608977
C	1.779091	1.229083	2.474762
H	0.999822	0.613243	2.933350
H	2.609601	0.563743	2.216832
H	2.140636	1.927362	3.233199

L90 – Hexene

Electronic Energy: -1663.27919258
Enthalpy: -1662.697335
Free Energy: -1662.785291

C	1.660239	-1.209091	-0.497643
N	1.941358	0.072759	-0.085719
P	0.635071	1.230173	-0.237757
C	3.349420	0.337676	0.254607
Cr	-1.483215	-0.195753	-0.605603
H	-4.089728	-0.093831	-1.716957
H	-2.980593	-0.838416	-0.449516
H	-2.598237	2.325830	-0.640669

H	-2.435362	1.587328	-2.299188
C	-3.568369	0.390034	-0.884433
C	-2.619924	1.414612	-1.238262
C	-2.474521	-1.863458	0.460745
C	-4.412580	0.538037	0.372326
C	-4.721280	-0.791076	1.059053
C	-3.458314	-1.486036	1.565908
H	-2.826582	-2.715131	-0.132425
H	-1.495715	-2.145520	0.866931
H	-3.880321	1.194896	1.078149
H	-5.341989	1.060704	0.115784
H	-5.407538	-0.621706	1.894409
H	-5.251324	-1.451256	0.357741
H	-2.961753	-0.821873	2.288494
H	-3.728638	-2.386905	2.131423
C	3.852008	-0.754859	1.182522
C	3.762129	-2.105891	0.503895
C	0.782931	-3.414739	-1.230483
C	1.977001	-3.478323	-0.592870
N	2.468391	-2.246377	-0.173115
H	3.950656	0.367378	-0.666133
H	3.422548	1.314988	0.726568
H	4.888921	-0.561231	1.466318
H	3.254742	-0.753109	2.101732
H	3.860257	-2.924968	1.220179
H	4.552582	-2.222491	-0.246594
H	2.584141	-4.350754	-0.383377
H	0.271596	-4.279506	-1.630911
P	0.283643	-1.728204	-1.472198
C	1.280602	2.526154	-1.444407
C	0.411116	1.901246	1.519280
C	1.817099	1.738829	-2.643980
H	2.730655	1.184733	-2.408346
H	1.080986	1.025486	-3.032897
H	2.055508	2.437935	-3.452807
C	-0.383202	0.816265	2.256109
H	-1.395394	0.702987	1.842208
H	0.116881	-0.159738	2.227442
H	-0.502913	1.091671	3.310065
C	0.097291	3.374906	-1.917446
H	-0.382867	3.935606	-1.111703
H	0.461145	4.105496	-2.648175
H	-0.664503	2.767355	-2.410161
C	2.371059	3.446099	-0.898297
H	2.677698	4.134281	-1.694444
H	2.023555	4.062330	-0.064239
H	3.270019	2.910621	-0.583284
C	1.691810	2.174466	2.305010
H	2.366159	2.878121	1.810233
H	1.418660	2.617575	3.269589
H	2.240604	1.255004	2.525733
C	-0.431710	3.175429	1.462768
H	-1.350798	3.044936	0.882371
H	-0.728703	3.448063	2.481669
H	0.118993	4.024958	1.049499

L90 – Octene

Electronic Energy: -1741.88565794
Enthalpy: -1741.241771
Free Energy: -1741.333347

C	1.880994	-1.307204	-0.258125
N	2.138621	0.048939	-0.265096
P	0.800895	1.134703	0.038903
C	4.196047	-1.866345	-1.009209
C	4.247087	-0.412491	-1.420658

C	3.553716	0.442123	-0.376546
C	1.086404	-3.663055	-0.195777
C	2.382864	-3.527170	-0.574612
N	2.827766	-2.214040	-0.616228
H	3.606896	1.493825	-0.645556
H	4.050522	0.323991	0.598265
H	5.287221	-0.097582	-1.530259
H	3.754806	-0.276667	-2.391206
H	4.491378	-2.530896	-1.824398
H	4.864179	-2.059494	-0.161786
Cr	-1.426272	-0.273874	0.563530
C	-2.976551	-1.839003	0.397565
C	-2.851893	-1.367854	-1.053967
C	-4.118173	-0.755082	-1.634817
C	-4.653733	0.445532	-0.868040
C	-2.714225	1.347624	0.534421
C	-3.628509	1.558278	-0.661619
H	-4.030295	-1.902611	0.662869
H	-2.013490	-0.652081	-1.270174
H	-4.884840	-1.537331	-1.684136
H	-5.525770	0.830647	-1.406877
H	-2.075060	2.225237	0.690386
H	-2.510681	-2.814089	0.532083
H	-2.515945	-2.224839	-1.648771
H	-3.914488	-0.461271	-2.672618
H	-5.031029	0.124592	0.114312
H	-3.323377	1.255080	1.445752
H	-3.045136	1.690854	-1.588043
H	-4.165563	2.509710	-0.531704
C	-1.510512	-0.417465	2.620928
H	-1.658180	0.589989	3.005955
H	-0.642324	-0.950981	3.003221
C	-2.673593	-1.177414	2.306933
H	-3.633800	-0.679607	2.408583
H	-2.692867	-2.224895	2.592102
H	0.580845	-4.614836	-0.108639
H	3.091856	-4.301509	-0.839047
P	0.374965	-2.087171	0.169178
C	0.645964	2.083843	-1.592794
C	1.375803	2.232129	1.465713
C	-0.061656	1.112980	-2.544490
H	0.448367	0.143896	-2.607446
H	-1.100106	0.940573	-2.241436
H	-0.088057	1.537744	-3.554208
C	1.886943	1.276520	2.547314
H	1.146017	0.509390	2.797704
H	2.812161	0.769719	2.260327
H	2.092727	1.844387	3.461193
C	-0.225849	3.323013	-1.394149
H	0.283874	4.102333	-0.820211
H	-0.463640	3.749587	-2.375351
H	-1.176465	3.097399	-0.902732
C	1.968102	2.498864	-2.236580
H	2.566789	1.635342	-2.539884
H	1.744337	3.063984	-3.148639
H	2.576928	3.147957	-1.601432
C	2.444431	3.273792	1.135632
H	2.115681	3.982710	0.370768
H	2.650855	3.856322	2.041001
H	3.395523	2.839938	0.820203
C	0.144206	2.961158	2.014072
H	0.444919	3.551414	2.886683
H	-0.300374	3.654632	1.295212
H	-0.631657	2.263888	2.340485

L91 – Hexene

Electronic Energy: -1810.86678181
Enthalpy: -1810.349388
Free Energy: -1810.438792

C	1.876533	-1.296468	-0.261471
N	2.069387	0.056161	-0.180783
P	0.602449	0.993205	-0.214747
C	4.201792	-1.768727	0.411673
Cr	-1.429343	-0.405609	-0.501738
H	-3.764330	0.208854	-1.982098
H	-3.028693	-0.740798	-0.597488
H	-2.101367	2.246004	-0.450185
H	-1.794277	1.646115	-2.147523
C	-3.326106	0.546880	-1.037410
C	-2.181648	1.415631	-1.154942
C	-2.839311	-1.899630	0.346374
C	-4.345064	0.796181	0.067058
C	-4.952196	-0.481011	0.640811
C	-3.900097	-1.366249	1.305712
H	-3.247592	-2.648622	-0.341888
H	-2.019143	-2.376731	0.892542
H	-3.852135	1.355629	0.876211
H	-5.129508	1.454492	-0.324129
H	-5.729475	-0.221592	1.366121
H	-5.455783	-1.042776	-0.158737
H	-3.414296	-0.787470	2.106742
H	-4.387735	-2.209977	1.810912
C	4.471950	-0.388112	-0.155615
C	3.373751	0.582447	0.239748
C	1.127521	-3.656486	-0.416655
C	2.429247	-3.507984	-0.062143
N	2.848836	-2.184015	0.032033
H	4.282154	-1.773401	1.504961
H	4.903812	-2.508222	0.020229
H	5.432349	-0.021944	0.213055
H	4.540221	-0.445024	-1.247758
H	3.516547	1.554582	-0.244046
H	3.373445	0.748410	1.326576
H	3.164657	-4.278601	0.130478
H	0.650385	-4.616492	-0.557174
P	0.381726	-2.081837	-0.751089
C	1.037590	2.321292	-1.366987
C	0.510830	3.609742	-1.208687
C	1.794247	2.020317	-2.507717
C	0.753869	4.585542	-2.170569
H	-0.081484	3.853104	-0.329946
C	2.035812	3.001630	-3.463306
H	2.196030	1.017966	-2.642072
C	1.516044	4.283591	-3.296261
H	0.348125	5.583778	-2.037750
H	2.629081	2.763692	-4.341048
H	1.704241	5.047204	-4.044785
C	0.490953	1.761673	1.425407
C	1.370129	2.768134	1.851125
C	-0.485319	1.284662	2.311039
C	1.273964	3.276356	3.142062
H	2.119049	3.160230	1.166466
C	-0.580307	1.795979	3.600894
H	-1.177949	0.505444	1.985316
C	0.301589	2.791101	4.015554
H	1.955883	4.056268	3.466888
H	-1.341839	1.421892	4.278305
H	0.228403	3.193936	5.021211

L91 – Octene
Electronic Energy: -1889.47469908

Enthalpy: -1888.896501
Free Energy: -1888.990289

C	1.983250	-1.269362	-0.133116
N	2.006272	0.076014	-0.434246
P	0.663916	1.019454	0.123918
C	4.251669	-1.598342	-1.087589
C	4.007322	-0.274538	-1.782793
C	3.271471	0.684611	-0.865366
C	1.581688	-3.650607	0.417423
C	2.778030	-3.417756	-0.181303
N	3.003387	-2.084263	-0.492628
H	3.031844	1.613791	-1.391071
H	3.884567	0.941888	0.010588
H	4.963012	0.161489	-2.081787
H	3.420326	-0.432857	-2.694207
H	4.611193	-2.358179	-1.785143
H	4.999162	-1.493821	-0.292071
Cr	-1.343607	-0.434271	0.678250
C	-2.833398	-1.938358	0.164532
C	-2.448720	-1.402222	-1.219675
C	-3.576619	-0.711750	-1.972217
C	-4.168722	0.494904	-1.257030
C	-2.473081	1.297887	0.469508
C	-3.135076	1.554038	-0.873207
H	-3.913335	-2.067810	0.204001
H	-1.562591	-0.707160	-1.255540
H	-4.360547	-1.452310	-2.170545
H	-4.934338	0.931217	-1.907052
H	-1.828568	2.141085	0.762186
H	-2.346411	-2.893584	0.363519
H	-2.045322	-2.247192	-1.789095
H	-3.194279	-0.398038	-2.952131
H	-4.700938	0.167738	-0.350746
H	-3.245078	1.226984	1.249388
H	-2.385043	1.639805	-1.674559
H	-3.627806	2.537264	-0.843603
C	-1.866668	-0.582287	2.659680
H	-2.037172	0.432648	3.014158
H	-1.132073	-1.163444	3.214969
C	-2.966830	-1.280462	2.074926
H	-3.898730	-0.731956	1.961539
H	-3.110194	-2.322048	2.347522
H	1.250516	-4.630304	0.733523
H	3.558179	-4.126707	-0.428030
P	0.693381	-2.139549	0.679472
C	0.337907	2.090775	-1.301340
C	0.391849	1.535155	-2.588035
C	-0.141433	3.396492	-1.135994
C	-0.003154	2.283986	-3.691304
H	0.747829	0.514877	-2.719984
C	-0.539348	4.139162	-2.244264
H	-0.205665	3.833837	-0.142819
C	-0.470094	3.586273	-3.520236
H	0.051314	1.850306	-4.685379
H	-0.904499	5.152538	-2.108061
H	-0.781204	4.168803	-4.382125
C	1.324935	2.081464	1.435310
C	2.132980	3.196975	1.168634
C	1.081362	1.707623	2.763981
C	2.678509	3.927566	2.218060
H	2.325153	3.496455	0.140659
C	1.632037	2.441463	3.809904
H	0.461395	0.837601	2.971931
C	2.427057	3.551640	3.536821
H	3.298818	4.793377	2.006801

H	1.436892	2.149059	4.837086
H	2.852021	4.127732	4.353379

L92 – Hexene
Electronic Energy: -1524.16765091
Enthalpy: -1523.723640
Free Energy: -1523.802646

N	2.295904	0.327318	0.486210
C	1.948395	1.643775	0.354662
P	1.137604	-0.912295	0.122867
H	3.044787	0.165482	1.152440
C	2.061376	-2.076979	-0.959072
C	3.326624	-2.611152	-0.301114
H	4.034854	-1.803368	-0.086726
H	3.125194	-3.148766	0.630482
H	3.832106	-3.308273	-0.975465
C	0.920817	-1.717079	1.775479
C	0.293899	-3.101002	1.677903
H	-0.738310	-3.052862	1.315590
H	0.852421	-3.775947	1.022658
H	0.261951	-3.561396	2.669515
C	0.807973	3.721421	-0.305342
C	1.751448	3.807269	0.667526
Cr	-0.964853	0.179213	-0.572754
H	-3.100450	-0.670575	-2.268520
H	-2.538878	0.426042	-0.941878
H	-0.939814	-1.822111	-2.301797
H	-1.324876	-2.530188	-0.665634
C	-2.669920	-0.944157	-1.299998
C	-1.430526	-1.678877	-1.337779
C	-2.527154	1.580489	-0.017666
C	-3.693594	-1.278790	-0.223918
C	-4.440372	-0.065071	0.323590
C	-3.497295	0.946268	0.972065
H	-3.036358	2.233056	-0.735584
H	-1.765455	2.190644	0.487999
H	-4.399870	-2.013532	-0.627892
H	-3.173694	-1.781082	0.606300
H	-5.185036	-0.397194	1.052798
H	-5.001521	0.422562	-0.485715
H	-4.073459	1.734851	1.472033
H	-2.933435	0.444089	1.774001
H	1.357479	-2.904566	-1.126955
C	2.352977	-1.394007	-2.290676
H	2.831980	-2.095552	-2.978981
H	1.444181	-1.022760	-2.776957
H	3.034073	-0.546702	-2.158205
H	1.932617	-1.815287	2.193724
C	0.101179	-0.782171	2.657828
H	0.552085	0.210816	2.754583
H	-0.916185	-0.656019	2.256243
H	-0.004700	-1.192848	3.666085
H	2.021310	4.732558	1.163211
H	0.208530	4.497685	-0.757952
N	2.381052	2.643377	1.052675
S	0.757328	2.083129	-0.897465

L92– Octene
Electronic Energy: -1602.78086010
Enthalpy: -1602.275572
Free Energy: -1602.358802

N	2.401449	0.062219	0.340307
C	2.079731	1.396819	0.270420
P	1.214874	-1.135083	-0.057031

C	2.086902	-2.265786	-1.217890
C	2.520500	-1.497058	-2.458321
H	1.655168	-1.110142	-3.008591
H	3.173997	-0.654978	-2.212605
H	3.070592	-2.155730	-3.136503
C	0.989910	-2.057731	1.534565
C	1.147027	3.564270	-0.389296
C	1.868163	3.525583	0.762823
Cr	-0.858941	0.087983	-0.884676
C	-2.293405	1.715281	-0.992116
C	-2.069384	1.591664	0.521215
C	-3.288270	1.140251	1.313600
C	-3.876245	-0.197465	0.885088
C	-2.063048	-1.497520	-0.360803
C	-2.881876	-1.358038	0.908971
H	-3.358663	1.828656	-1.183652
H	-1.202506	0.948012	0.849804
H	-4.052036	1.922603	1.233104
H	-4.723575	-0.417353	1.542121
H	-1.406539	-2.378952	-0.321611
H	-1.762151	2.580330	-1.392417
H	-1.704316	2.564678	0.871009
H	-3.012130	1.092087	2.374314
H	-4.301957	-0.112269	-0.126104
H	-2.729595	-1.642116	-1.222923
H	-2.231353	-1.267484	1.792955
H	-3.438032	-2.293876	1.064870
C	-1.061014	-0.230054	-2.896779
H	-1.198002	-1.302492	-3.027079
H	-0.239989	0.210627	-3.462371
C	-2.219904	0.574539	-2.676058
H	-3.170424	0.061660	-2.550480
H	-2.303997	1.511168	-3.218613
C	2.184308	-2.925098	1.912361
H	3.109191	-2.341971	1.994034
H	2.013798	-3.387649	2.889019
H	2.359618	-3.732846	1.197145
H	0.121900	-2.706046	1.346183
C	0.630737	-1.072060	2.642470
H	-0.186841	-0.397990	2.360002
H	0.313686	-1.610874	3.539459
H	1.485603	-0.446266	2.920200
H	2.980241	-2.632420	-0.694004
C	1.172798	-3.438217	-1.555415
H	0.881449	-4.017378	-0.672723
H	0.256507	-3.096796	-2.051797
H	1.676365	-4.124186	-2.242313
H	2.045857	4.387833	1.394714
H	0.663719	4.404139	-0.867746
N	2.375379	2.305821	1.146261
S	1.173619	1.994826	-1.137964
H	3.081898	-0.139001	1.067623

L93 – Hexene

Electronic Energy: -1524.16792938
Enthalpy: -1523.723405
Free Energy: -1523.801211

N	2.361755	0.348490	0.530728
C	2.069096	1.569672	0.271660
P	1.157863	-0.810143	0.159560
C	2.033788	-2.027224	-0.907104
C	3.270706	-2.600619	-0.227484
H	3.986341	-1.809328	0.015526
H	3.033372	-3.135704	0.696907
H	3.770091	-3.308159	-0.896333

C	0.885003	-1.601541	1.810405
C	0.212962	-2.962915	1.702968
H	-0.800767	-2.878337	1.293907
H	0.770492	-3.667043	1.078170
H	0.118761	-3.411757	2.696353
C	0.992385	3.829702	-0.256453
C	2.169664	3.901537	0.387240
Cr	-1.039199	0.190777	-0.392678
H	-3.038955	-0.485613	-2.303617
H	-2.610930	0.420813	-0.778080
H	-0.840274	-1.561438	-2.370387
H	-1.267552	-2.484691	-0.856712
C	-2.654155	-0.882801	-1.359025
C	-1.382529	-1.560935	-1.424171
C	-2.690282	1.418029	0.308982
C	-3.726473	-1.403550	-0.410267
C	-4.557385	-0.309309	0.256633
C	-3.703195	0.618714	1.119635
H	-3.170720	2.176940	-0.318161
H	-1.965161	1.941356	0.950425
H	-4.376332	-2.093966	-0.960693
H	-3.236782	-2.005211	0.370683
H	-5.336888	-0.770011	0.870419
H	-5.080210	0.279508	-0.510109
H	-4.345496	1.305606	1.684874
H	-3.179791	0.014696	1.876954
H	1.298695	-2.826834	-1.076261
C	2.370766	-1.373656	-2.242877
H	2.800820	-2.109329	-2.928418
H	1.490314	-0.941238	-2.730973
H	3.109604	-0.575364	-2.114399
H	1.882758	-1.710838	2.255942
C	0.053402	-0.639112	2.652303
H	0.518441	0.348599	2.741128
H	-0.947959	-0.504584	2.207577
H	-0.098096	-1.026005	3.664365
H	2.677879	4.802692	0.700369
H	0.364534	4.639614	-0.593830
N	2.763141	2.678955	0.646563
S	0.618576	2.158391	-0.645742
H	3.612019	2.577544	1.185915

L93 – Octene

Electronic Energy: -1602.78148684
Enthalpy: -1602.276529
Free Energy: -1602.361502

N	2.301625	0.097475	0.676379
C	2.256785	1.318525	0.276860
P	1.138950	-1.008077	0.114810
C	2.058795	-2.092980	-1.063163
C	2.514380	-1.283761	-2.269541
H	1.660121	-0.886720	-2.830247
H	3.154276	-0.443161	-1.984861
H	3.089783	-1.914555	-2.953964
C	0.832716	-2.031650	1.625932
C	1.810272	3.648076	-0.658308
C	2.770269	3.601190	0.281338
Cr	-0.959885	0.093237	-0.785340
C	-2.443794	1.675166	-0.827294
C	-2.313011	1.416374	0.676875
C	-3.560149	0.857641	1.347117
C	-4.050752	-0.466548	0.777622
C	-2.105760	-1.576710	-0.451671
C	-2.996015	-1.573201	0.775700
H	-3.494487	1.794876	-1.084580

H	-1.452907	0.756539	0.990723
H	-4.352704	1.611739	1.275133
H	-4.923864	-0.780297	1.358377
H	-1.401022	-2.419069	-0.437120
H	-1.897292	2.575087	-1.116779
H	-1.999766	2.357686	1.142932
H	-3.351209	0.735881	2.417471
H	-4.415819	-0.320040	-0.250006
H	-2.715768	-1.684997	-1.359996
H	-2.396196	-1.514775	1.697536
H	-3.505849	-2.546010	0.833041
C	-1.051670	-0.073856	-2.829163
H	-1.138653	-1.138546	-3.039849
H	-0.219885	0.432870	-3.318246
C	-2.246454	0.672026	-2.607488
H	-3.185437	0.125100	-2.568568
H	-2.335078	1.650137	-3.070416
C	2.048766	-2.843022	2.053044
H	2.914827	-2.195149	2.222874
H	1.838322	-3.364739	2.991953
H	2.328050	-3.602292	1.317427
H	0.018149	-2.714497	1.343038
C	0.349308	-1.125044	2.752358
H	-0.502679	-0.500518	2.455191
H	0.031732	-1.721269	3.612864
H	1.150645	-0.457347	3.084363
H	2.945595	-2.439923	-0.515664
C	1.200686	-3.285242	-1.465554
H	0.881186	-3.884732	-0.606499
H	0.301614	-2.964099	-2.005017
H	1.760057	-3.946407	-2.134262
H	3.342633	4.433593	0.665244
H	1.453532	4.507618	-1.204385
N	3.021048	2.334582	0.770319
S	1.214825	2.036568	-1.009792
H	3.686778	2.141123	1.505706

L94 – Hexene
Electronic Energy: -1563.46869356
Enthalpy: -1562.994405
Free Energy: -1563.075438

N	2.322902	0.360929	0.488975
C	1.901418	1.653235	0.335799
P	1.210734	-0.908489	0.069881
C	2.248817	-2.048623	-0.940823
C	2.573675	-1.385592	-2.273982
H	1.665989	-1.208149	-2.862681
H	3.085141	-0.426987	-2.144591
H	3.227547	-2.030292	-2.867983
C	0.795075	-1.788273	1.646053
C	0.001260	-0.837229	2.535233
H	0.606725	0.016701	2.858978
H	-0.885828	-0.438196	2.018556
H	-0.354409	-1.349303	3.433851
C	0.697547	3.684558	-0.366521
C	1.638781	3.818109	0.603638
Cr	-0.955891	0.157568	-0.574993
H	-3.207244	-0.767590	-2.079042
H	-2.555442	0.383483	-0.848692
H	-1.081775	-1.958353	-2.176301
H	-1.352475	-2.542725	-0.467365
C	-2.722980	-0.986320	-1.121872
C	-1.495498	-1.739400	-1.191377
C	-2.505250	1.613128	-0.021537
C	-3.689617	-1.239110	0.026043

C	-4.427261	0.011957	0.494649
C	-3.472053	1.076056	1.029067
H	-3.015935	2.211922	-0.784632
H	-1.738976	2.254907	0.431126
H	-4.403179	-2.011745	-0.283494
H	-3.128314	-1.666591	0.870927
H	-5.147937	-0.260162	1.271342
H	-5.015264	0.426841	-0.335905
H	-4.040895	1.911383	1.456380
H	-2.903078	0.649924	1.869067
H	3.181917	-2.180208	-0.374644
C	1.596177	-3.414514	-1.116954
H	2.267656	-4.068228	-1.680871
H	1.386214	-3.912638	-0.165669
H	0.661429	-3.351001	-1.680816
H	0.113590	-2.575315	1.288688
C	1.945627	-2.452833	2.390672
H	2.586135	-3.052180	1.735881
H	2.573251	-1.721864	2.906465
H	1.546491	-3.126685	3.154710
H	1.875324	4.760200	1.084821
H	0.064893	4.431014	-0.824470
N	2.308246	2.683987	1.008373
S	0.710056	2.038948	-0.936741
C	3.562276	0.177034	1.246358
H	3.425886	0.424589	2.303763
H	3.889036	-0.859169	1.158309
H	4.338044	0.829447	0.839171

L94 – Octene

Electronic Energy: -1642.08227322
Enthalpy: -1641.547130
Free Energy: -1641.633116

N	2.486180	0.110850	0.084257
C	2.165971	1.444681	0.011362
P	1.247745	-1.068275	-0.193088
C	2.025658	-2.269971	-1.352481
C	2.489500	-1.553907	-2.613157
H	1.648043	-1.085752	-3.137098
H	3.228123	-0.775925	-2.399659
H	2.948407	-2.266993	-3.304024
C	1.000355	-1.957916	1.419440
C	1.190288	3.623054	-0.571142
C	2.136872	3.606724	0.404907
Cr	-0.887163	0.113159	-0.897238
C	-2.412041	1.668991	-0.960927
C	-2.124678	1.555918	0.543408
C	-3.282562	1.046989	1.390530
C	-3.814747	-0.325579	1.001866
C	-2.021978	-1.517605	-0.365523
C	-2.754047	-1.425712	0.960742
H	-3.489036	1.706233	-1.113852
H	-1.216493	0.954381	0.836423
H	-4.090851	1.785646	1.339414
H	-4.604475	-0.591560	1.711439
H	-1.351231	-2.386951	-0.396635
H	-1.958263	2.572218	-1.370816
H	-1.793018	2.545004	0.880256
H	-2.955692	1.025483	2.437766
H	-4.307314	-0.271910	0.019439
H	-2.744320	-1.653893	-1.182944
H	-2.047371	-1.290806	1.795982
H	-3.241622	-2.391522	1.157841
C	-1.127845	-0.215158	-2.901861
H	-1.240878	-1.290563	-3.031681

H	-0.333987	0.245905	-3.489480
C	-2.306024	0.555338	-2.655917
H	-3.238415	0.012627	-2.524068
H	-2.424501	1.491249	-3.193435
C	2.060216	-2.982125	1.805174
H	3.025219	-2.519559	2.028771
H	1.741162	-3.507189	2.710920
H	2.216811	-3.742220	1.034873
H	0.056064	-2.495533	1.244179
C	0.763508	-0.935711	2.526448
H	-0.007010	-0.202132	2.260972
H	0.431303	-1.437449	3.439810
H	1.674961	-0.379624	2.769368
H	2.898599	-2.695521	-0.837390
C	1.033331	-3.387400	-1.657119
H	0.695119	-3.913545	-0.757924
H	0.147078	-2.997674	-2.171206
H	1.493032	-4.129616	-2.315753
H	2.466065	4.489907	0.940110
H	0.635703	4.456549	-0.978102
N	2.678508	2.388820	0.740153
S	1.020447	2.020791	-1.224122
C	3.764622	-0.213315	0.720660
H	4.523504	0.491326	0.375757
H	3.710510	-0.150466	1.812654
H	4.063939	-1.222620	0.431048

L95 – Hexene

Electronic Energy: -1563.47379826
Enthalpy: -1562.999741
Free Energy: -1563.081111

N	2.294121	0.370533	0.652173
C	1.992917	1.587103	0.363582
P	1.138689	-0.811891	0.212862
C	2.076250	-2.007259	-0.826449
C	3.294435	-2.564279	-0.101403
H	3.981587	-1.761500	0.183217
H	3.028085	-3.117278	0.804384
H	3.838382	-3.251610	-0.756496
C	0.826615	-1.617389	1.848782
C	0.162844	-2.979870	1.716231
H	-0.840862	-2.896849	1.282880
H	0.739498	-3.675420	1.099025
H	0.046877	-3.438300	2.702943
C	0.925272	3.815404	-0.244020
C	2.043223	3.902819	0.497535
Cr	-1.053873	0.170450	-0.397901
H	-3.020935	-0.485248	-2.344891
H	-2.617580	0.415381	-0.802381
H	-0.830651	-1.577759	-2.375883
H	-1.288069	-2.501426	-0.871159
C	-2.657073	-0.890348	-1.395385
C	-1.389037	-1.576451	-1.439191
C	-2.705095	1.401781	0.286317
C	-3.750987	-1.405610	-0.469133
C	-4.586360	-0.306862	0.185269
C	-3.743315	0.609488	1.071767
H	-3.163814	2.174821	-0.339838
H	-1.981195	1.907464	0.944011
H	-4.395962	-2.088858	-1.034138
H	-3.281375	-2.013805	0.318967
H	-5.383564	-0.763140	0.779284
H	-5.086631	0.290369	-0.590004
H	-4.391819	1.299848	1.625442
H	-3.242506	-0.002963	1.837393

H	1.361656	-2.818159	-1.028027
C	2.454400	-1.341274	-2.144787
H	2.927861	-2.064875	-2.814358
H	1.586494	-0.924841	-2.667637
H	3.170571	-0.528585	-1.983262
H	1.813053	-1.725953	2.319079
C	-0.024960	-0.657071	2.671926
H	0.438254	0.331026	2.769267
H	-1.015844	-0.523964	2.204586
H	-0.199448	-1.043217	3.680630
H	2.504935	4.813207	0.855815
H	0.317596	4.616854	-0.634265
N	2.649510	2.696186	0.809118
S	0.618354	2.142215	-0.670028
C	3.790892	2.556182	1.700120
H	3.474369	2.154716	2.666602
H	4.517597	1.872529	1.259803
H	4.249861	3.533615	1.842711

L95 – Octene
Electronic Energy: -1642.08758041
Enthalpy: -1641.553227
Free Energy: -1641.642060

N	2.286974	0.089256	0.698499
C	2.221913	1.322028	0.327460
P	1.124566	-1.011821	0.131345
C	2.055371	-2.105357	-1.030220
C	2.520900	-1.304806	-2.238536
H	1.671306	-0.932961	-2.822834
H	3.138508	-0.448001	-1.952642
H	3.122569	-1.933969	-2.901556
C	0.797217	-2.029995	1.642776
C	1.738201	3.660315	-0.533592
C	2.708810	3.593259	0.394642
Cr	-0.965116	0.096103	-0.783892
C	-2.453248	1.676623	-0.836475
C	-2.332567	1.411273	0.667613
C	-3.584999	0.849190	1.325187
C	-4.072506	-0.470433	0.742406
C	-2.116044	-1.574740	-0.475656
C	-3.019596	-1.578939	0.742310
H	-3.502993	1.786846	-1.101845
H	-1.475117	0.749618	0.986403
H	-4.376327	1.604521	1.252443
H	-4.951342	-0.786671	1.313131
H	-1.412497	-2.418129	-0.458614
H	-1.914062	2.583584	-1.116323
H	-2.022527	2.350253	1.140413
H	-3.384262	0.719655	2.396192
H	-4.428221	-0.316250	-0.287410
H	-2.716246	-1.676888	-1.391301
H	-2.429049	-1.528349	1.670584
H	-3.531986	-2.551056	0.787271
C	-1.028169	-0.054119	-2.829563
H	-1.110895	-1.116796	-3.051348
H	-0.188962	0.457913	-3.299992
C	-2.227361	0.688298	-2.619202
H	-3.165402	0.138828	-2.598628
H	-2.311573	1.669404	-3.076653
C	2.010020	-2.833696	2.092421
H	2.868491	-2.179101	2.275834
H	1.786897	-3.355429	3.028428
H	2.307223	-3.592052	1.363002
H	-0.010592	-2.716997	1.350248
C	0.294253	-1.122630	2.760008

H	-0.553856	-0.499244	2.450045
H	-0.035366	-1.718185	3.616483
H	1.089709	-0.453601	3.104261
H	2.938049	-2.443607	-0.470466
C	1.207265	-3.304669	-1.432037
H	0.884728	-3.901168	-0.572094
H	0.310708	-2.991686	-1.980367
H	1.775446	-3.966451	-2.092728
H	3.274851	4.422870	0.796067
H	1.371194	4.532078	-1.052622
N	2.992993	2.319897	0.854149
S	1.161133	2.055071	-0.926396
C	3.962954	2.014124	1.892591
H	3.458735	1.631668	2.783779
H	4.660700	1.254477	1.535725
H	4.509276	2.922356	2.143365

L96 – Hexene
Electronic Energy: -1205.8761
Enthalpy: -1205.351119
Free Energy: -1205.433218

N	2.147688	0.638555	0.612968
C	1.424452	1.783855	0.528713
N	0.153667	1.755851	0.238667
P	1.353061	-0.823958	0.111484
H	3.126479	0.7035	0.861761
C	2.49746	-1.529121	-1.151369
C	3.860434	-1.913255	-0.591496
H	4.396433	-1.042982	-0.194463
H	3.795086	-2.661574	0.203681
H	4.487163	-2.334184	-1.383284
C	1.437439	-1.912214	1.599915
C	1.056154	-3.342396	1.23773
H	0.024892	-3.396056	0.869561
H	1.709740	-3.777810	0.475647
H	1.114645	-3.981797	2.123093
C	-0.347681	3.140449	0.093938
C	2.002830	3.152620	0.689952
H	2.636158	3.240341	1.577088
C	0.743759	4.019552	0.732299
H	0.865465	4.970524	0.209513
H	0.483688	4.247181	1.769152
H	2.645298	3.367430	-0.173753
H	-1.291466	3.221771	0.645332
C	-0.609106	3.429364	-1.373765
H	-1.299878	2.691071	-1.80105
H	-1.058711	4.416920	-1.509211
H	0.318020	3.395454	-1.957189
Cr	-0.873646	0.021139	-0.365384
H	-2.800600	-0.591661	-2.358776
H	-2.482278	0.048817	-0.663486
H	-0.516123	-1.432430	-2.56493
H	-0.831528	-2.595703	-1.20017
C	-2.382739	-1.094372	-1.480208
C	-1.044982	-1.615188	-1.628416
C	-2.694426	0.856314	0.571994
C	-3.405380	-1.885698	-0.674034
C	-4.377934	-1.012098	0.11333
C	-3.664123	-0.164053	1.163958
H	-3.226298	1.671331	0.065075
H	-2.075061	1.307933	1.355578
H	-3.948445	-2.554597	-1.352111
H	-2.863997	-2.537879	0.028551
H	-5.128503	-1.645764	0.595561
H	-4.929040	-0.357489	-0.57712

H	-4.400551	0.349297	1.79552
H	-3.117126	-0.838857	1.840379
H	1.977539	-2.435903	-1.492873
C	2.611349	-0.562796	-2.325778
H	3.154160	-1.029453	-3.152274
H	1.631557	-0.251985	-2.705761
H	3.162400	0.340821	-2.043297
H	2.475241	-1.887205	1.960273
C	0.514064	-1.339434	2.668146
H	0.758176	-0.303016	2.920716
H	-0.532297	-1.365036	2.331584
H	0.572446	-1.929000	3.587744

L96 – Octene
Electronic Energy = -1284.481713
Enthalpy = -1283.894623
Free Energy = -1283.97938

N	-2.098475	0.806659	-0.670634
C	-1.246347	1.861439	-0.777590
N	-0.001530	1.794053	-0.406592
P	-1.528004	-0.697122	-0.023640
H	-3.035023	0.924602	-1.035914
C	-2.768139	-1.099713	1.289658
C	-4.179171	-1.305622	0.751465
H	-4.572964	-0.393882	0.286853
H	-4.247307	-2.116004	0.020621
H	-4.854880	-1.554879	1.574967
C	-1.860522	-1.888577	-1.399578
C	0.626057	3.120648	-0.609713
C	-1.685263	3.191274	-1.309726
H	-2.290616	3.098456	-2.215759
C	-0.345326	3.889675	-1.524807
H	-0.375071	4.955891	-1.290348
H	-0.038205	3.792671	-2.569572
H	-2.315143	3.689739	-0.562559
H	1.589693	2.967255	-1.112305
C	0.867929	3.800821	0.725836
H	1.490620	3.183620	1.380598
H	1.377858	4.758264	0.587465
H	-0.075859	3.993783	1.247888
Cr	0.822376	-0.055615	0.508268
C	2.869963	0.655625	0.259000
C	2.601994	-0.055144	-1.072037
C	3.503264	-1.249812	-1.352433
C	3.452227	-2.349253	-0.299777
C	1.279405	-2.035014	1.012075
C	2.047316	-2.872052	-0.002075
H	3.844237	0.351888	0.637445
H	1.546159	-0.409930	-1.241814
H	4.531442	-0.884762	-1.460377
H	4.095507	-3.167853	-0.639200
H	0.335396	-2.534552	1.278855
H	2.855601	1.738276	0.133543
H	2.675710	0.693550	-1.869421
H	3.225008	-1.669623	-2.327787
H	3.902172	-1.990540	0.638198
H	1.856773	-1.990406	1.947753
H	1.487747	-2.956440	-0.949362
H	2.131267	-3.905582	0.365674
C	0.843729	0.536488	2.473521
H	0.503332	-0.319030	3.054609
H	0.274410	1.457673	2.596713
C	2.238200	0.636686	2.200844
H	2.869021	-0.183948	2.531079

H	2.717379	1.607968	2.291144
C	-0.936485	-1.603943	-2.576361
H	0.106677	-1.829939	-2.322468
H	-1.203089	-2.234900	-3.429397
H	-0.988228	-0.562518	-2.909334
H	-2.899356	-1.705506	-1.710248
C	-1.728762	-3.329025	-0.917129
H	-2.415266	-3.569934	-0.099873
H	-1.948464	-4.016559	-1.739134
H	-0.710557	-3.546148	-0.577127
H	-2.402960	-2.046084	1.713536
C	-2.736706	-0.032539	2.376750
H	-1.743788	0.083688	2.817821
H	-3.047335	0.942412	1.985010
H	-3.428984	-0.295871	3.181460

L97 – Hexene
Electronic Energy = -1166.560118
Enthalpy = -1166.064489
Free Energy = -1166.143109

N	-2.134581	0.900395	0.323150
C	-1.374870	1.996693	0.080239
N	-0.108141	1.890742	-0.218479
P	-1.381819	-0.650641	0.080565
H	-3.124629	1.031752	0.488487
C	-1.396575	-1.452515	1.744593
C	-2.754599	-1.422681	2.427998
H	-3.068633	-0.394863	2.640000
H	-3.536413	-1.903629	1.831818
H	-2.709883	-1.948095	3.386488
C	-2.645559	-1.532312	-0.937305
C	0.445243	3.247122	-0.384927
C	-1.883420	3.401208	0.157066
H	-2.875390	3.516984	-0.288290
C	-0.769543	4.159385	-0.563714
H	-0.608343	5.164655	-0.172356
H	-1.012920	4.252431	-1.626254
H	-1.971877	3.691719	1.211706
H	1.134182	3.269441	-1.233480
Cr	0.903986	0.046659	-0.425866
H	2.519354	-0.009931	-0.679636
H	0.594806	-2.007897	-2.128807
H	0.941884	-2.688827	-0.473474
C	2.440699	-1.295255	-1.207427
C	1.119133	-1.877001	-1.182269
C	-2.675527	-0.948441	-2.344843
H	-2.870932	0.128055	-2.346294
H	-1.726942	-1.118898	-2.865773
H	-3.463155	-1.425776	-2.934961
H	-3.611820	-1.337304	-0.447528
C	-2.396194	-3.036002	-0.949560
H	-2.469412	-3.485817	0.044520
H	-3.141749	-3.526329	-1.582016
H	-1.412167	-3.281083	-1.362323
H	-1.117647	-2.494439	1.532686
C	-0.295252	-0.827030	2.594422
H	-0.211899	-1.333714	3.560303
H	0.684214	-0.899157	2.098590
H	-0.490871	0.232456	2.795105
C	3.521539	-1.829943	-0.275171
H	3.034593	-2.300686	0.591931
H	4.062531	-2.631374	-0.791522
C	4.488737	-0.756941	0.216815
H	4.977397	-0.278080	-0.643904
H	5.288639	-1.224435	0.799298

C	3.784459	0.300404	1.064697
H	3.320191	-0.201960	1.926414
H	4.524706	0.989593	1.491014
C	2.719226	1.097402	0.312570
H	2.100766	1.666153	1.015824
H	3.166039	1.816373	-0.385189
H	2.812990	-1.019739	-2.199820
H	1.028092	3.509701	0.507948

L97 – Octene

Electronic Energy = -1245.1663
Enthalpy = -1244.608979
Free Energy = -1244.692987

N	-2.206657	0.603851	-0.628701
C	-1.572600	1.806886	-0.627812
N	-0.326204	1.935316	-0.275670
P	-1.368740	-0.805340	-0.064750
H	-3.159080	0.578351	-0.969954
C	-2.510009	-1.511033	1.209472
C	-3.861652	-1.929303	0.644214
H	-4.416046	-1.072102	0.244041
H	-3.785141	-2.683075	-0.144125
H	-4.478887	-2.356425	1.440214
C	-1.461787	-1.962572	-1.504396
C	0.022607	3.362789	-0.327408
C	-2.268386	3.083934	-0.987736
H	-2.889743	2.990320	-1.882625
C	-1.087627	4.040432	-1.138001
H	-1.305831	5.052782	-0.795240
H	-0.793722	4.105897	-2.189466
H	-2.939286	3.366356	-0.166347
H	1.009598	3.495225	-0.781307
Cr	0.824951	0.223055	0.510592
C	2.704324	1.312855	0.284625
C	2.606056	0.554357	-1.043500
C	3.733160	-0.440067	-1.287169
C	3.856078	-1.527344	-0.228322
C	1.622138	-1.642237	1.006265
C	2.566702	-2.310863	0.016437
H	3.712399	1.207228	0.680941
H	1.649693	-0.012457	-1.224956
H	4.673304	0.119074	-1.361097
H	4.659419	-2.205744	-0.534391
H	0.785376	-2.315295	1.248211
H	2.483010	2.370303	0.145818
H	2.545847	1.295380	-1.849045
H	3.576786	-0.906489	-2.268372
H	4.188545	-1.086531	0.723536
H	2.155229	-1.489665	1.957345
H	2.065615	-2.487061	-0.951107
H	2.830936	-3.314216	0.381826
C	0.705933	0.800187	2.479180
H	0.546279	-0.108228	3.057376
H	-0.041373	1.582936	2.604072
C	2.051701	1.186384	2.215805
H	2.834734	0.515975	2.559606
H	2.312983	2.237348	2.301297
C	-0.586339	-1.449922	-2.640049
H	0.476040	-1.511087	-2.372979
H	-0.727996	-2.060817	-3.536385
H	-0.810817	-0.412685	-2.909158
H	-2.510911	-1.961179	-1.833346
C	-1.065413	-3.374088	-1.084573
H	-1.727818	-3.794447	-0.322243
C	-2.510009	-1.511033	1.209472

C	-3.861652	-1.929303	0.644214
H	-4.416046	-1.072102	0.244041
H	-3.785141	-2.683075	-0.144125
H	-4.478887	-2.356425	1.440214
C	-1.461787	-1.962572	-1.504396
C	0.022607	3.362789	-0.327408
C	-2.268386	3.083934	-0.987736
H	-2.889743	2.990320	-1.882625
C	-1.087627	4.040432	-1.138001
H	-1.305831	5.052782	-0.795240
H	-0.793722	4.105897	-2.189466
H	-2.939286	3.366356	-0.166347
H	1.009598	3.495225	-0.781307
Cr	0.824951	0.223055	0.510592
C	2.704324	1.312855	0.284625
C	2.606056	0.554357	-1.0435
C	3.73316	-0.440067	-1.287169
C	3.856078	-1.527344	-0.228322
C	1.622138	-1.642237	1.006265
C	2.566702	-2.310863	0.016437
H	3.712399	1.207228	0.680941
H	1.649693	-0.012457	-1.224956
H	4.673304	0.119074	-1.361097
H	4.659419	-2.205744	-0.534391
H	0.785376	-2.315295	1.248211
H	2.48301	2.370303	0.145818
H	2.545847	1.29538	-1.849045
H	3.576786	-0.906489	-2.268372
H	4.188545	-1.086531	0.723536
H	2.155229	-1.489665	1.957345
H	2.065615	-2.487061	-0.951107
H	2.830936	-3.314216	0.381826
C	0.705933	0.800187	2.47918
H	0.546279	-0.108228	3.057376
H	-0.041373	1.582936	2.604072
C	2.051701	1.186384	2.215805
H	2.834734	0.515975	2.559606
H	2.312983	2.237348	2.301297
C	-0.586339	-1.449922	-2.640049
H	0.47604	-1.511087	-2.372979
H	-0.727996	-2.060817	-3.536385
H	-0.810817	-0.412685	-2.909158
H	-2.510911	-1.961179	-1.833346
C	-1.065413	-3.374088	-1.084573
H	-1.727818	-3.794447	-0.322243

L98 – Hexene

Electronic Energy = -1245.189706
Enthalpy = -1244.63443
Free Energy = -1244.716616

N	1.904345	0.796425	0.732695
C	2.082394	-0.552589	0.573234
N	1.116795	-1.254320	0.054215
P	0.487198	1.544524	0.072010
H	2.678181	1.321188	1.121963
C	-0.150597	2.553096	1.479899
C	-1.245285	3.501735	1.006603
H	-0.907570	4.185193	0.221320
H	-1.597802	4.112967	1.842332
H	-2.111272	2.949449	0.623921
C	1.136556	2.725742	-1.189753
C	2.008237	3.829990	-0.607308
H	1.473494	4.455209	0.113521
H	2.365271	4.487721	-1.405473
H	2.897678	3.424544	-0.110672

C	1.295629	-2.693054	-0.241402
Cr	-0.783718	-0.432789	-0.453115
H	-2.873681	-1.130097	-2.234078
H	-2.135758	-1.356688	-0.552179
H	-2.262346	1.709455	-1.334224
H	-1.450019	0.804852	-2.690211
C	-2.741562	-0.414637	-1.415441
C	-1.928472	0.741958	-1.711155
C	-1.761644	-2.032828	0.719578
C	-3.969721	-0.256641	-0.527386
C	-4.230509	-1.455936	0.380963
C	-3.094501	-1.681015	1.377914
H	-1.771000	-3.051057	0.310468
H	-0.938216	-1.981145	1.443928
H	-3.835024	0.640361	0.096135
H	-4.842122	-0.056974	-1.160766
H	-5.170864	-1.306520	0.920523
H	-4.370657	-2.358888	-0.230764
H	-2.976808	-0.765974	1.978478
H	-3.373307	-2.466319	2.092202
C	2.737386	-3.168600	-0.125361
C	3.408201	-1.094779	1.021822
H	4.165904	-0.762875	0.298626
C	3.395490	-2.609571	1.120580
H	2.746137	-4.262661	-0.128679
H	3.300172	-2.849424	-1.014261
H	3.675819	-0.620930	1.972834
H	2.836545	-2.920796	2.011700
H	4.414196	-2.985750	1.240034
H	0.687888	-3.235549	0.498830
C	0.729963	-2.968021	-1.625508
H	0.801927	-4.030982	-1.872028
H	-0.330467	-2.691804	-1.694445
H	1.280761	-2.405338	-2.387922
H	0.697512	3.139322	1.861635
H	0.227417	3.171012	-1.619116
C	1.856273	1.939878	-2.280520
H	2.782841	1.494130	-1.901657
H	1.237810	1.131416	-2.687018
H	2.127231	2.598807	-3.110106
C	-0.649260	1.618808	2.574692
H	-1.501160	1.021260	2.222021
H	0.125622	0.926471	2.918158
H	-0.992515	2.189530	3.442501

L98 – Octene
Electronic Energy = -1323.790836
Enthalpy = -1323.172711
Free Energy = -1323.257838

N	1.456261	1.657256	-0.479102
C	2.166063	0.483251	-0.543071
N	1.598948	-0.635771	-0.204197
P	-0.202217	1.704178	-0.010435
H	1.943180	2.491970	-0.781723
C	-0.242722	3.047290	1.265640
C	0.172164	4.406530	0.713642
H	1.204796	4.395720	0.345125
H	-0.473471	4.759715	-0.094524
H	0.133579	5.156353	1.509530
C	-1.027903	2.429437	-1.500760
C	2.374558	-1.891473	-0.308638
H	1.681571	-2.628054	-0.736732
C	2.760487	-2.367346	1.084060
H	1.888597	-2.419416	1.741776
H	3.210239	-3.363622	1.041528

H	3.480295	-1.690592	1.555313
C	3.575319	-1.794613	-1.244637
C	3.571591	0.658612	-1.053333
H	3.491533	0.940941	-2.112265
C	4.425268	-0.586508	-0.903061
H	4.016221	1.523853	-0.549311
H	4.151996	-2.722205	-1.180164
H	3.223897	-1.712512	-2.281486
H	4.801257	-0.663661	0.123450
H	5.303581	-0.518591	-1.549224
Cr	-0.551539	-0.682022	0.537673
C	-0.767492	-2.864563	0.423943
C	-1.100638	-2.403363	-1.001271
C	-2.507583	-2.755060	-1.467636
C	-3.623483	-2.215312	-0.583585
C	-2.598424	-0.314353	0.787996
C	-3.551804	-0.710957	-0.331447
H	-1.537604	-3.555083	0.762392
H	-0.970025	-1.304194	-1.218333
H	-2.581690	-3.846565	-1.537006
H	-4.578542	-2.474043	-1.052857
H	-2.712224	0.755335	1.019095
H	0.198347	-3.368502	0.451575
H	-0.344449	-2.820021	-1.677248
H	-2.637047	-2.374817	-2.489108
H	-3.620195	-2.737189	0.384864
H	-2.893092	-0.840800	1.707811
H	-3.291072	-0.202730	-1.274780
H	-4.563091	-0.350847	-0.090295
C	-0.263471	-0.812496	2.562652
H	-0.974018	-0.129477	3.024824
H	0.786983	-0.642085	2.800798
C	-0.698131	-2.150872	2.328052
H	-1.731111	-2.380531	2.573245
H	-0.015490	-2.965906	2.552884
C	-0.989005	1.435048	-2.652880
H	-1.610760	0.558038	-2.436130
H	-1.384096	1.892641	-3.564714
H	0.025978	1.088228	-2.872186
H	-0.427394	3.308888	-1.774284
C	-2.451459	2.874714	-1.186596
H	-2.498068	3.616511	-0.383598
H	-2.903223	3.328002	-2.073953
H	-3.082750	2.027790	-0.898866
H	-1.296150	3.092049	1.576210
C	0.606310	2.654882	2.468217
H	0.264899	1.728011	2.933873
H	1.657512	2.524616	2.188531
H	0.566955	3.441148	3.227710

L99 – Hexene

Electronic Energy = -1205.872909
Enthalpy = -1205.346709
Free Energy = -1205.426652

N	-2.103858	-0.27367	0.525355
C	-1.992483	1.075210	0.319207
N	-0.842644	1.555791	-0.060649
P	-0.775325	-1.308411	0.114704
H	-3.008535	-0.624292	0.815292
C	-0.404935	-2.204599	1.686993
C	0.536903	-3.372768	1.420166
H	0.115919	-4.111971	0.732113
H	0.764940	-3.891136	2.356023
H	1.490566	-3.028227	1.002674
C	-1.516923	-2.543279	-1.039863

C	-2.597806	-3.404808	-0.399902
H	-2.231348	-3.985740	0.451059
H	-2.993391	-4.115356	-1.131804
H	-3.446572	-2.800418	-0.058384
C	-0.703406	2.995014	-0.328597
Cr	0.861912	0.370548	-0.474718
H	2.939162	0.652442	-2.398575
H	2.314157	1.094259	-0.713284
H	1.912432	-2.005582	-1.344614
H	1.177002	-1.027012	-2.694947
C	2.723334	0.004236	-1.543470
C	1.718501	-1.010712	-1.747645
C	2.134273	1.848439	0.552892
C	3.941989	-0.334924	-0.692109
C	4.435762	0.813778	0.183463
C	3.383387	1.255700	1.198148
H	2.341859	2.826237	0.101816
H	1.337044	1.996195	1.292147
H	3.683302	-1.186122	-0.043744
H	4.745055	-0.688942	-1.349521
H	5.347320	0.505885	0.705043
H	4.719425	1.667816	-0.448124
H	3.103311	0.384406	1.811135
H	3.816399	1.979810	1.900249
C	-2.012545	3.725615	-0.552274
C	-3.242714	1.876469	0.537260
H	-3.936172	1.617848	-0.274871
C	-2.986771	3.374608	0.557439
H	-1.819637	4.801118	-0.590530
H	-2.438117	3.444537	-1.524216
H	-3.724290	1.530907	1.458379
H	-2.564224	3.667947	1.526072
H	-3.931053	3.913664	0.450252
H	-0.163196	3.444373	0.515805
H	-1.360777	-2.585053	2.073887
H	-0.663888	-3.178637	-1.318773
C	-2.022812	-1.832586	-2.290005
H	-2.901659	-1.217866	-2.067509
H	-1.262074	-1.183005	-2.735865
H	-2.320881	-2.562217	-3.047888
C	0.190341	-1.223776	2.689583
H	1.154350	-0.835506	2.331756
H	-0.466571	-0.369897	2.881551
H	0.376852	-1.719172	3.646975
H	-0.041770	3.097175	-1.197559

L99 – Octene

Electronic Energy = -1284.478873
Enthalpy = -1283.891199
Free Energy = -1283.976881

N	2.017413	0.769287	-0.623736
C	2.200274	-0.591297	-0.598561
N	1.239163	-1.356241	-0.177947
P	0.574167	1.509607	-0.029893
H	2.773840	1.319571	-1.011192
C	1.155668	2.687262	1.275562
C	2.153777	3.717825	0.762714
H	3.089812	3.246713	0.440753
H	1.767008	4.315555	-0.067270
H	2.414307	4.412680	1.566565
C	0.073258	2.581226	-1.453876
C	1.469881	-2.801312	-0.071721
H	0.926546	-3.291488	-0.893280
C	2.925239	-3.226536	-0.092617
C	3.557875	-1.048184	-1.058953

H	3.817692	-0.506356	-1.975479
C	3.636704	-2.552656	-1.250435
H	4.284589	-0.718336	-0.304230
H	3.407734	-2.945268	0.852738
H	2.980620	-4.316227	-0.163937
H	4.680909	-2.865959	-1.322899
H	3.155976	-2.835699	-2.194949
Cr	-0.723273	-0.534599	0.528535
C	-1.800917	-2.424872	0.199918
C	-2.020062	-1.686108	-1.123215
C	-3.475894	-1.376436	-1.446957
C	-4.196235	-0.533966	-0.403192
C	-2.396373	0.627565	0.990547
C	-3.489344	0.776271	-0.059088
H	-2.752484	-2.823325	0.546426
H	-1.460531	-0.718389	-1.251301
H	-4.003533	-2.326865	-1.589200
H	-5.206725	-0.332345	-0.774149
H	-2.028983	1.617646	1.301215
H	-1.097753	-3.245895	0.069268
H	-1.556411	-2.280826	-1.918666
H	-3.511083	-0.860312	-2.415279
H	-4.332447	-1.115846	0.520643
H	-2.831901	0.182590	1.898196
H	-3.089420	1.219201	-0.987110
H	-4.241342	1.497059	0.294882
C	-0.415852	-1.049216	2.493105
H	-0.763323	-0.211805	3.095357
H	0.622442	-1.344212	2.644437
C	-1.366133	-2.056081	2.153909
H	-2.392580	-1.890691	2.469350
H	-1.059608	-3.096701	2.216076
C	-0.407591	1.719477	-2.613635
H	-1.353957	1.222049	-2.368703
H	-0.589096	2.338329	-3.497356
H	0.320150	0.951035	-2.894258
H	0.984944	3.112114	-1.765201
C	-0.977381	3.602034	-1.031917
H	-0.605717	4.304746	-0.280402
H	-1.293197	4.190306	-1.898579
H	-1.872077	3.116632	-0.626756
H	0.234727	3.203289	1.583574
C	1.703980	1.921113	2.472023
H	0.965394	1.235709	2.895014
H	2.592388	1.338643	2.203489
H	2.000890	2.618139	3.261072
H	0.986984	-3.137189	0.854797

L100 – Hexene
Electronic Energy = -1245.180316
Enthalpy = -1244.624604
Free Energy = -1244.707166

N	-1.641686	1.390171	0.09363
C	-2.145869	0.185138	-0.306452
N	-1.313888	-0.780429	-0.593429
P	0.074929	1.615776	0.126166
H	-2.303911	2.114111	0.341940
C	0.322316	3.229622	-0.730206
C	-0.295673	4.412308	0.004436
H	-1.382846	4.309877	0.099741
H	0.120261	4.553678	1.006063
H	-0.115466	5.334894	-0.555313
C	0.452492	1.886250	1.914216
C	1.888916	2.367465	2.077248
H	2.601552	1.623508	1.700162

H	2.082313	3.310971	1.557650
H	2.117749	2.523960	3.135429
C	-1.879014	-2.069678	-1.018607
Cr	0.801226	-0.567202	-0.611089
H	2.869424	-1.533632	-2.306341
H	1.795091	-1.851547	-0.841079
H	2.176720	0.812515	-2.401377
H	2.974360	1.095202	-0.787261
C	2.805566	-1.000131	-1.352447
C	2.439817	0.393439	-1.429103
C	1.036747	-2.612232	0.196582
C	3.849457	-1.429667	-0.327984
C	3.578773	-2.790673	0.306978
C	2.263340	-2.808682	1.082854
H	0.863628	-3.486328	-0.443285
H	0.129236	-2.468510	0.796048
H	4.836854	-1.416877	-0.804388
H	3.886502	-0.669833	0.467388
H	4.406775	-3.051711	0.973358
H	3.558474	-3.566918	-0.471487
H	2.169573	-3.748064	1.642933
H	2.299213	-2.014953	1.846119
C	-2.612891	-2.825406	0.086234
C	-3.641908	0.068992	-0.346660
H	-4.078504	1.061989	-0.206069
C	-4.212494	-0.910761	0.685964
H	-5.277160	-0.687087	0.804073
H	-2.607981	-3.891543	-0.165451
H	-2.041895	-2.728342	1.020025
H	-3.752742	-0.719042	1.664623
H	-3.938300	-0.255097	-1.353263
H	-2.549276	-1.923017	-1.878806
C	-4.051645	-2.373522	0.298053
H	-4.522617	-3.000509	1.062211
H	-4.615069	-2.553012	-0.628573
H	1.415351	3.347159	-0.744082
H	-0.239309	2.656885	2.281448
C	0.206275	0.584773	2.668265
H	-0.805905	0.194963	2.515330
H	0.916148	-0.191170	2.350520
H	0.347176	0.728985	3.743449
C	-0.176546	3.120212	-2.166493
H	0.271561	2.273615	-2.696891
H	-1.264458	2.998422	-2.199961
H	0.069080	4.028469	-2.723671
H	-1.041871	-2.668676	-1.386236

L100 – Octene
Electronic Energy = -1323.784952
Enthalpy = -1323.167208
Free Energy = -1323.256544

N	-1.238937	1.799148	-0.254581
P	0.455110	1.610415	0.064842
H	-1.696761	2.698022	-0.170513
C	1.172459	3.064559	-0.822415
C	0.612330	2.011850	1.867448
Cr	0.708753	-0.737791	-0.606140
C	0.822090	-2.935923	-0.714614
C	0.519954	-2.669988	0.763543
C	1.594208	-3.189581	1.719671
C	3.004400	-2.668371	1.453800
C	2.738185	-0.712754	-0.186312
C	3.120566	-1.161631	1.221277
H	1.854790	-3.259393	-0.834467
H	0.391288	-1.594890	1.069540

H	1.593776	-4.284959	1.686759
H	3.626779	-2.961472	2.306026
H	3.105622	0.305605	-0.375092
H	0.151360	-3.703188	-1.095490
H	-0.466951	-3.074639	1.012150
H	1.290685	-2.915815	2.738742
H	3.441071	-3.184436	0.587618
H	3.231419	-1.354337	-0.933630
H	2.519436	-0.628356	1.979652
H	4.158954	-0.868984	1.434550
C	0.901664	-0.603254	-2.643829
H	1.896279	-0.254620	-2.914900
H	0.070600	0.003748	-3.000237
C	0.687206	-2.008824	-2.528891
H	1.476866	-2.677879	-2.856863
H	-0.309292	-2.373035	-2.767024
C	-0.125447	0.961471	2.689099
H	-1.202627	0.980750	2.486617
H	0.234233	-0.054103	2.489780
H	0.008275	1.150839	3.758087
C	1.036511	2.895774	-2.329168
H	1.670777	2.082051	-2.694103
H	0.006130	2.685605	-2.632281
H	1.351367	3.811350	-2.838535
C	-4.507719	-1.068366	0.574209
C	-3.240632	-1.908856	0.478977
C	-2.384532	-1.619826	-0.752333
C	-4.283224	0.435896	0.633583
C	-3.514359	0.989729	-0.572288
H	-5.138151	-1.291700	-0.297848
H	-2.618927	-1.770315	1.375616
H	-3.027076	-1.502949	-1.639027
H	-3.756138	0.710123	1.557449
H	-3.673702	2.067810	-0.661655
H	-5.086323	-1.379279	1.450356
H	-3.521935	-2.967747	0.462445
H	-1.744155	-2.483631	-0.957708
H	-5.253327	0.940535	0.677352
H	-3.910734	0.541305	-1.492462
N	-1.496676	-0.463809	-0.599549
C	-2.040217	0.713561	-0.496903
H	1.690595	1.920839	2.065645
H	0.568864	3.927721	-0.504945
C	2.619323	3.303068	-0.406324
H	3.012542	4.180497	-0.927785
H	2.730708	3.486670	0.666561
H	3.260363	2.456132	-0.672541
C	0.150771	3.419296	2.221684
H	-0.912699	3.560348	1.995407
H	0.270668	3.593528	3.295178
H	0.716704	4.198665	1.703934

L101 – Hexene

Electronic Energy = -1747.782601
Enthalpy = -1747.006205
Free Energy = -1747.11759

N	0.037806	-1.809776	-0.103677
C	-0.524084	-0.570376	0.071583
N	0.281070	0.451846	0.235316
P	1.747336	-2.002386	0.132521
H	-0.598195	-2.595239	-0.030688
C	-0.210103	1.784105	0.378841
C	0.099554	2.447534	1.584531
C	-0.870468	2.450701	-0.669255

C	-0.297345	3.774171	1.740411
C	-1.241594	3.784754	-0.469267
C	-0.967350	4.443948	0.720550
H	-0.074500	4.282593	2.675285
H	-1.750105	4.307145	-1.276201
H	-1.265960	5.479557	0.851993
C	-1.997768	-0.533407	0.032738
C	-2.753219	0.257340	0.909870
C	-2.672959	-1.310514	-0.917164
C	-4.135981	0.262674	0.824610
C	-4.059738	-1.280550	-1.004965
C	-4.824249	-0.493321	-0.137424
H	-2.260074	0.858197	1.667452
H	-2.103902	-1.909907	-1.625545
H	-4.697255	0.873619	1.526905
H	-4.544822	-1.878933	-1.769126
C	0.827018	1.740847	2.689015
H	1.874586	1.515351	2.427769
H	0.862766	2.356056	3.591262
H	0.361586	0.784691	2.953566
C	-1.188223	1.792414	-1.976362
H	-2.208504	1.390133	-1.989244
H	-1.119692	2.512249	-2.796493
H	-0.514978	0.960849	-2.206003
C	-6.347724	-0.439985	-0.191837
C	-6.914628	-1.284763	-1.330566
C	-6.799672	1.012847	-0.389837
H	-6.466342	1.664619	0.423709
H	-6.416822	1.427097	-1.328182
H	-7.892810	1.065567	-0.423072
H	-6.562285	-0.945477	-2.310435
H	-8.006192	-1.213811	-1.335136
H	-6.659481	-2.344386	-1.225267
C	-6.911350	-0.965883	1.135311
H	-6.576477	-0.368336	1.988987
H	-8.005821	-0.933775	1.120144
H	-6.610615	-2.003230	1.315182
C	1.807235	-3.256149	1.488057
C	2.310397	-2.850107	-1.409816
Cr	2.422840	0.309502	0.197310
H	4.541107	1.705465	1.421671
H	3.388930	1.617393	-0.019533
H	4.125092	-0.615174	2.037336
H	4.734352	-1.156722	0.405697
C	4.462029	0.991898	0.594514
C	4.220409	-0.381019	0.976289
C	2.471586	2.106037	-1.104095
C	5.404963	1.291994	-0.565283
C	4.983812	2.498132	-1.400051
C	3.633474	2.276398	-2.079416
H	2.198154	3.051621	-0.620145
H	1.576688	1.738571	-1.621221
H	6.416648	1.430824	-0.166514
H	5.452258	0.404823	-1.214133
H	5.748878	2.705974	-2.154415
H	4.934320	3.391143	-0.760532
H	3.419374	3.108249	-2.762723
H	3.710376	1.383597	-2.718618
C	1.299490	-2.632636	2.782614
H	1.940970	-1.802994	3.102589
H	0.276817	-2.253798	2.690410
H	1.300727	-3.375336	3.585670
C	1.535106	-4.120612	-1.726856
H	1.926382	-4.585022	-2.636971
H	1.601122	-4.866829	-0.929242
H	0.475868	-3.905476	-1.908663

H	3.360846	-3.104725	-1.210015
C	2.268578	-1.843656	-2.554955
H	1.242029	-1.524983	-2.770775
H	2.859432	-0.945433	-2.328014
H	2.674850	-2.281116	-3.471453
H	1.121619	-4.062207	1.187002
C	3.209667	-3.831074	1.645850
H	3.215063	-4.575996	2.446884
H	3.569226	-4.327473	0.739880
H	3.933262	-3.056190	1.918437

L101 – Octene

Electronic Energy = -1826.384896
Enthalpy = -1825.546992
Free Energy = -1825.66202

N	0.090781	1.779044	0.139257
C	0.652312	0.530770	0.226732
N	-0.127133	-0.511978	0.375202
P	-1.621991	2.007101	0.131143
H	0.731255	2.561647	0.198564
C	0.430309	-1.818066	0.221387
C	0.513582	-2.661321	1.345548
C	0.803079	-2.276673	-1.057415
C	0.982670	-3.963898	1.173434
C	1.259682	-3.591817	-1.184552
C	1.351817	-4.432949	-0.083095
H	1.059609	-4.611969	2.043239
H	1.544584	-3.951057	-2.170695
H	1.710339	-5.450923	-0.201665
C	2.127564	0.515580	0.117700
C	2.922264	-0.278327	0.955344
C	2.764008	1.337118	-0.821177
C	4.302770	-0.241824	0.848270
C	4.149910	1.348722	-0.934366
C	4.952131	0.562255	-0.101074
H	2.459387	-0.908298	1.707891
H	2.167527	1.950069	-1.495015
H	4.893398	-0.855354	1.523645
H	4.604936	1.983852	-1.687513
C	0.117859	-2.164570	2.700103
H	-0.967077	-2.031015	2.777457
H	0.416124	-2.865277	3.483329
H	0.558177	-1.188047	2.932387
C	0.709995	-1.394887	-2.264086
H	1.557488	-0.701048	-2.331809
H	0.707171	-1.986814	-3.182845
H	-0.196424	-0.778875	-2.255220
C	6.475843	0.560795	-0.175932
C	6.999601	1.461515	-1.292191
C	6.972426	-0.868831	-0.428389
H	6.667938	-1.558415	0.365118
H	6.593375	-1.262872	-1.376774
H	8.066352	-0.884949	-0.472709
H	6.645403	1.143434	-2.278519
H	8.092847	1.427018	-1.312634
H	6.711230	2.507891	-1.147710
C	7.039463	1.059982	1.161417
H	6.732269	0.425741	1.998873
H	8.134202	1.060092	1.133505
H	6.711069	2.081772	1.378204
C	-1.827989	3.361851	1.371013
C	-1.950627	2.799831	-1.511094
Cr	-2.432772	-0.292614	0.385596
C	-2.833815	-2.433131	0.345030
C	-2.620432	-2.130739	-1.137407

C	-3.827654	-2.374352	-2.030157
C	-5.078848	-1.598240	-1.645546
C	-4.334936	0.375486	-0.198863
C	-4.871031	-0.088592	-1.545446
H	-3.712901	-3.062849	0.467331
H	-2.238310	-1.096204	-1.377757
H	-4.040353	-3.449813	-2.024903
H	-5.856084	-1.824092	-2.383324
H	-4.336118	1.474691	-0.160366
H	-1.961358	-2.928639	0.774543
H	-1.756556	-2.721065	-1.466362
H	-3.549546	-2.123408	-3.062130
H	-5.467116	-1.967415	-0.684376
H	-5.028282	0.055730	0.592724
H	-4.216962	0.243319	-2.368677
H	-5.833503	0.409217	-1.734832
C	-2.970747	-0.187112	2.383007
H	-3.682263	0.633071	2.457260
H	-2.080820	-0.103989	3.006544
C	-3.476426	-1.479466	2.087897
H	-4.539078	-1.571511	1.882129
H	-3.060441	-2.340845	2.602652
C	-1.407992	2.915618	2.765128
H	-2.123568	2.206623	3.189140
H	-0.419050	2.446155	2.776939
H	-1.369479	3.778911	3.436062
C	-1.295983	4.163136	-1.683570
H	-0.205865	4.102233	-1.579165
H	-1.497097	4.552034	-2.686331
H	-1.664783	4.904522	-0.969598
H	-3.044341	2.916042	-1.534595
C	-1.540196	1.835081	-2.617147
H	-0.453941	1.689701	-2.633474
H	-2.009413	0.850129	-2.502865
H	-1.834070	2.225003	-3.595929
H	-1.147360	4.159414	1.037236
C	-3.258315	3.888899	1.347479
H	-3.365310	4.712792	2.059065
H	-3.555640	4.266505	0.363829
H	-3.974467	3.112849	1.639581

L102 - Hexene

Electronic Energy = -1973.976222
Enthalpy = -1973.20536
Free Energy = -1973.322202

N	0.030673	1.362213	0.144572
C	0.832849	0.276069	-0.102361
N	0.243710	-0.861023	-0.385020
P	-1.672122	1.220154	-0.144212
H	0.486082	2.266467	0.187103
C	0.971759	-2.076885	-0.541713
C	1.638400	-2.675243	0.542876
C	0.894961	-2.714138	-1.797027
C	2.252325	-3.914122	0.332009
C	1.531405	-3.942725	-1.962163
C	2.208851	-4.543173	-0.904602
H	2.767061	-4.387765	1.164590
H	1.489975	-4.430636	-2.932951
H	2.695408	-5.503699	-1.044638
C	2.282406	0.510512	0.001834
C	2.779659	1.353858	1.008245
C	3.190179	-0.081831	-0.882332
C	4.142249	1.570708	1.133239
C	4.553007	0.157607	-0.756384
C	5.063273	0.978144	0.256074

H	2.097503	1.806648	1.724703
H	2.832231	-0.723322	-1.681143
H	4.500674	2.209767	1.936473
H	5.226095	-0.310505	-1.466876
C	1.711103	-2.032541	1.893735
H	0.858826	-1.373796	2.091151
H	1.735982	-2.789851	2.681578
H	2.617197	-1.423938	2.004809
C	0.151137	-2.079376	-2.934162
H	0.428886	-1.030020	-3.086778
H	0.330751	-2.613381	-3.870251
H	-0.939685	-2.089957	-2.776989
C	-2.444989	1.384203	1.487791
C	-3.828592	1.606260	1.556923
C	-1.728244	1.121813	2.661573
C	-4.478676	1.578318	2.785726
C	-2.386249	1.096670	3.887950
C	-3.759405	1.320537	3.951485
H	-4.394062	1.812225	0.649741
H	-0.655561	0.948652	2.615404
H	-5.548096	1.760359	2.832787
H	-1.823455	0.902315	4.796111
H	-4.269304	1.297555	4.909687
C	-2.098145	2.703905	-1.083176
C	-2.412551	3.918546	-0.459369
C	-2.079162	2.622578	-2.482344
C	-2.697942	5.038958	-1.232467
C	-2.361792	3.747846	-3.248480
C	-2.671590	4.953947	-2.623140
H	-2.441748	3.983455	0.625681
H	-1.847473	1.674062	-2.964164
H	-2.942648	5.979322	-0.748098
H	-2.349077	3.682151	-4.331986
H	-2.899479	5.830579	-3.222128
C	6.554792	1.240373	0.439548
C	7.402125	0.516871	-0.604629
C	6.976857	0.756074	1.833205
H	6.434429	1.275457	2.629589
H	6.799180	-0.317553	1.953839
H	8.044858	0.938752	1.990456
H	7.277874	-0.569860	-0.554049
H	8.461242	0.730956	-0.433807
H	7.165521	0.838746	-1.624225
C	6.819918	2.747756	0.329419
H	6.528931	3.136162	-0.651897
H	6.275391	3.317157	1.089179
H	7.886133	2.954673	0.467923
Cr	-1.856619	-1.118538	-0.618866
H	-3.579477	-2.876252	-2.058214
H	-2.605019	-2.575320	-0.528945
H	-4.222745	0.020859	-1.404441
H	-3.228168	-0.570141	-2.812375
C	-3.685526	-2.087823	-1.305469
C	-3.527239	-0.732412	-1.775740
C	-1.827927	-2.870732	0.707930
C	-4.734268	-2.380330	-0.239199
C	-4.313781	-3.450698	0.764985
C	-3.079590	-3.035865	1.564605
H	-1.446977	-3.831983	0.340516
H	-1.014654	-2.404923	1.278675
H	-4.944557	-1.446916	0.304374
H	-5.671709	-2.663142	-0.733025
H	-5.145319	-3.655561	1.446555
H	-4.111664	-4.394517	0.238263
H	-3.300633	-2.086243	2.077520
H	-2.888251	-3.764715	2.363005

L102 - Octene
Electronic Energy = -2052.58073
Enthalpy = -2051.749282
Free Energy = -2051.870532

N	0.088945	-1.363975	-0.567776
C	0.862088	-0.229881	-0.514887
N	0.260329	0.931577	-0.528929
P	-1.577190	-1.288553	-0.118702
H	0.579614	-2.248427	-0.623440
C	0.999720	2.112830	-0.228348
C	1.239442	3.053328	-1.245704
C	1.375194	2.367468	1.105315
C	1.889133	4.243805	-0.913638
C	2.028536	3.568375	1.391598
C	2.288347	4.501056	0.393391
H	2.081447	4.972908	-1.697312
H	2.323934	3.771102	2.418387
H	2.793277	5.431383	0.635569
C	2.315673	-0.469686	-0.399310
C	3.261384	0.291185	-1.099898
C	2.774797	-1.490918	0.442942
C	4.613411	0.023594	-0.963065
C	4.135125	-1.737933	0.586866
C	5.085845	-0.992687	-0.117678
H	2.934642	1.079349	-1.770057
H	2.061439	-2.072583	1.025001
H	5.323457	0.620757	-1.530078
H	4.451941	-2.525714	1.262413
C	0.830827	2.764547	-2.656590
H	1.569098	2.141852	-3.178824
H	-0.112456	2.210943	-2.696044
H	0.722388	3.683433	-3.238591
C	1.059708	1.389113	2.193625
H	1.699075	0.498111	2.153095
H	1.195460	1.839296	3.179821
H	0.025352	1.025332	2.127099
C	6.586746	-1.236627	0.003215
C	6.909595	-2.408219	0.927477
C	7.253325	0.028398	0.560035
H	7.081152	0.897772	-0.082211
H	6.877338	0.273251	1.558652
H	8.336110	-0.115945	0.635832
H	6.560867	-2.235887	1.951046
H	7.992706	-2.554617	0.974864
H	6.469992	-3.346320	0.572087
C	7.163043	-1.538792	-1.386375
H	7.005699	-0.711740	-2.085349
H	8.242380	-1.709390	-1.318338
H	6.710338	-2.435353	-1.822133
Cr	-2.022356	1.086375	-0.415508
C	-2.139593	3.242439	-0.646425
C	-2.009371	3.084569	0.872490
C	-3.197084	3.614679	1.662693
C	-4.530803	2.972870	1.307861
C	-4.003634	0.736095	0.178146
C	-4.533810	1.449657	1.414007
H	-2.927919	3.959648	-0.865354
H	-1.813098	2.039220	1.257725
H	-3.249092	4.698578	1.506268
H	-5.296990	3.399343	1.963980
H	-4.142887	-0.349610	0.292905
H	-1.201333	3.586611	-1.082325
H	-1.073437	3.571192	1.172487

H	-2.997356	3.468736	2.731884
H	-4.823652	3.258003	0.286175
H	-4.618196	1.016792	-0.690184
H	-3.974687	1.148771	2.315402
H	-5.564447	1.115545	1.602899
C	-2.482924	0.816750	-2.408376
H	-3.292594	0.089216	-2.432073
H	-1.591580	0.548911	-2.976465
C	-2.819536	2.193556	-2.284194
H	-3.870299	2.439802	-2.156301
H	-2.272189	2.920925	-2.877610
C	-2.343866	-2.505287	-1.213550
C	-3.496516	-3.186693	-0.799881
C	-1.865878	-2.683388	-2.518664
C	-4.149386	-4.046429	-1.677683
C	-2.520248	-3.550183	-3.387272
C	-3.661886	-4.230679	-2.969197
H	-3.874677	-3.056434	0.211647
H	-0.977701	-2.149699	-2.848093
H	-5.037740	-4.576952	-1.348945
H	-2.137649	-3.693061	-4.393345
H	-4.170844	-4.905753	-3.650530
C	-1.653839	-2.009069	1.545771
C	-1.920777	-1.157938	2.624483
C	-1.386957	-3.364877	1.784312
C	-1.919841	-1.651059	3.925989
C	-1.382544	-3.853123	3.085563
C	-1.648815	-2.997379	4.154614
H	-2.138270	-0.105955	2.435793
H	-1.195603	-4.036094	0.949161
H	-2.135720	-0.987860	4.758029
H	-1.176584	-4.903479	3.268079
H	-1.649031	-3.384632	5.169019

L103 – Hexene

Electronic Energy = -1669.155994
Enthalpy = -1668.438517
Free Energy = -1668.544382

N	-0.068209	1.948327	-0.088046
C	0.470473	0.692445	-0.183695
N	-0.358927	-0.321787	-0.265066
P	-1.788905	2.131108	-0.183938
H	0.572648	2.727349	-0.177307
C	0.096228	-1.673393	-0.254828
C	0.703457	-2.236545	0.881793
C	-0.208529	-2.457475	-1.385454
C	1.039864	-3.593886	0.841040
C	0.152006	-3.803286	-1.383993
C	0.777827	-4.372140	-0.278061
H	1.507782	-4.039346	1.715770
H	-0.066895	-4.407608	-2.261072
H	1.048299	-5.423649	-0.286226
C	1.941571	0.615844	-0.148117
C	2.654385	1.451748	0.726277
C	2.659594	-0.276265	-0.951583
C	4.034635	1.369153	0.809824
C	4.045704	-0.335991	-0.871567
C	4.765132	0.471327	0.017046
H	2.116758	2.135834	1.379233
H	2.137994	-0.921918	-1.651264
H	4.557034	2.010268	1.515413
H	4.569810	-1.032742	-1.517372
C	0.988929	-1.438310	2.116535
H	0.301523	-0.593709	2.237018
H	0.907450	-2.064333	3.009009

H	2.004559	-1.023751	2.108133
C	-0.903749	-1.853368	-2.568124
H	-0.388427	-0.965520	-2.951643
H	-0.986232	-2.571166	-3.387404
H	-1.932234	-1.535704	-2.330438
C	6.281679	0.397530	0.164980
C	6.910610	-0.588945	-0.815988
C	6.614799	-0.051006	1.594939
H	6.224494	0.646378	2.343128
H	6.198758	-1.040348	1.811430
H	7.699700	-0.107175	1.731990
H	6.553135	-1.611942	-0.659002
H	7.996264	-0.601359	-0.682754
H	6.712503	-0.316060	-1.857945
C	6.887627	1.785579	-0.079672
H	6.509517	2.530841	0.627203
H	7.975488	1.747850	0.037547
H	6.673438	2.144469	-1.091485
C	-2.229847	2.851108	1.445019
H	-1.642017	3.761488	1.612839
H	-1.896028	2.121158	2.193152
C	-3.720997	3.116862	1.575941
H	-4.078722	3.841270	0.837374
H	-4.306067	2.199134	1.446992
H	-3.956295	3.517703	2.564365
C	-2.012696	3.478430	-1.402179
H	-3.094309	3.571168	-1.556446
H	-1.614932	3.096169	-2.348957
C	-1.399369	4.820464	-1.039977
H	-1.869738	5.261299	-0.156770
H	-0.323815	4.751178	-0.846568
H	-1.527965	5.528902	-1.861803
Cr	-2.483361	-0.154865	-0.378671
H	-4.575783	-1.608695	-1.615628
H	-3.486523	-1.430847	-0.128441
H	-4.678529	1.368105	-1.008455
H	-3.903888	0.594690	-2.465609
C	-4.508185	-0.797230	-0.883465
C	-4.149170	0.501043	-1.406021
C	-2.701923	-1.777642	1.094885
C	-5.544434	-0.878153	0.231417
C	-5.238889	-1.924068	1.299675
C	-3.915327	-1.644048	2.008409
H	-2.516537	-2.818388	0.802901
H	-1.790524	-1.418832	1.589222
H	-5.611050	0.108637	0.713495
H	-6.528219	-1.061737	-0.216528
H	-6.055377	-1.946603	2.028285
H	-5.207047	-2.924595	0.845139
H	-3.951109	-0.623135	2.423559
H	-3.803137	-2.309075	2.874568

L103 – Octene

Electronic Energy = -1747.759019
Enthalpy = -1746.980132
Free Energy = -1747.092218

N	-0.082671	1.936769	0.120113
C	-0.601739	0.665841	0.177091
N	0.229701	-0.341872	0.177137
P	1.624719	2.195094	0.243797
H	-0.740218	2.691497	0.275441
C	-0.248061	-1.682965	0.254989
C	-0.793559	-2.330638	-0.868383
C	-0.070306	-2.366271	1.474562
C	-1.144572	-3.678519	-0.749698

C	-0.435353	-3.711520	1.547502
C	-0.965990	-4.369051	0.442587
H	-1.563866	-4.185563	-1.615665
H	-0.304572	-4.240165	2.488742
H	-1.240595	-5.417318	0.511765
C	-2.078638	0.592872	0.165901
C	-2.788154	1.423661	-0.716412
C	-2.801615	-0.285159	0.979174
C	-4.169366	1.350234	-0.796749
C	-4.189349	-0.333400	0.904110
C	-4.905301	0.469733	0.009797
H	-2.246342	2.100174	-1.373882
H	-2.285329	-0.927472	1.685419
H	-4.687838	1.987752	-1.508665
H	-4.716651	-1.018332	1.560032
C	-1.022595	-1.606255	-2.157802
H	-0.275645	-0.826878	-2.334017
H	-1.005577	-2.295001	-3.006566
H	-2.001167	-1.109642	-2.168277
C	0.437276	-1.647081	2.686451
H	-0.311509	-0.950151	3.086258
H	0.687220	-2.346623	3.487693
H	1.324898	-1.041269	2.472515
C	-6.423568	0.409994	-0.129826
C	-7.058386	-0.547829	0.875474
C	-6.769065	-0.064739	-1.548392
H	-6.370082	0.609593	-2.312999
H	-6.369537	-1.065102	-1.744229
H	-7.855219	-0.106595	-1.680939
H	-6.714724	-1.578293	0.737811
H	-8.145046	-0.549542	0.749787
H	-6.849443	-0.255298	1.910016
C	-7.013368	1.809305	0.088391
H	-6.631241	2.535727	-0.635682
H	-8.102222	1.781084	-0.022367
H	-6.789960	2.187041	1.091336
C	1.813013	3.680087	-0.810287
H	1.068273	4.416001	-0.480969
C	3.209248	4.279598	-0.778851
H	3.526158	4.530620	0.238592
H	3.954161	3.598440	-1.199913
H	3.240550	5.201462	-1.364221
H	1.530547	3.386112	-1.826671
C	1.904288	2.803961	1.953267
H	2.993689	2.866999	2.074744
C	1.234505	4.114478	2.326861
H	1.615848	4.952178	1.735986
H	0.148972	4.072979	2.191832
H	1.416957	4.350548	3.378187
H	1.583396	1.988912	2.613680
Cr	2.429738	-0.011856	-0.398441
C	2.771205	-2.079126	-0.984832
C	3.173628	-2.092898	0.493147
C	4.624638	-2.469181	0.753450
C	5.640672	-1.537431	0.109895
C	4.416981	0.638743	-0.447835
C	5.424562	-0.064384	0.449622
H	3.527790	-2.598889	-1.568896
H	2.989688	-1.143497	1.077309
H	4.778393	-3.496462	0.402976
H	6.640715	-1.856924	0.421393
H	4.743907	0.564231	-1.496256
H	1.801504	-2.558507	-1.125094
H	2.484421	-2.770334	1.010922
H	4.787248	-2.487743	1.838381
H	5.618152	-1.656054	-0.983724

H	4.410463	1.711686	-0.210550
H	5.131258	0.026746	1.508870
H	6.390738	0.456471	0.379336
C	2.129504	0.546960	-2.366044
H	2.803186	1.380019	-2.559276
H	1.074159	0.745535	-2.557046
C	2.629036	-0.768815	-2.574472
H	3.668857	-0.860980	-2.874100
H	1.974510	-1.506525	-3.030271

L104 – Hexene
Electronic Energy = -1895.355485
Enthalpy = -1895.644335
Free Energy = -1894.757909

N	1.214234	-0.119363	-0.378309
C	0.769312	1.163294	-0.502497
N	-0.517158	1.380989	-0.434110
P	0.047438	-1.396120	-0.329892
H	2.216376	-0.274620	-0.421069
C	-1.051146	2.695402	-0.605074
C	-1.727216	2.972514	-1.809825
C	-1.014848	3.631395	0.444390
C	-2.347616	4.212335	-1.957351
C	-1.655323	4.860043	0.253299
C	-2.314284	5.153414	-0.932926
H	-2.865222	4.433826	-2.887631
H	-1.635518	5.589428	1.059619
H	-2.807110	6.112636	-1.058951
C	-1.803155	1.947335	-2.900365
H	-2.457368	1.103884	-2.627362
H	-2.216671	2.374375	-3.816743
H	-0.826447	1.514404	-3.143713
C	-0.311540	3.350266	1.737860
H	-0.255837	2.280372	1.961781
H	0.717308	3.733623	1.733313
H	-0.819734	3.840121	2.572449
C	0.721644	-2.672687	-1.416630
C	1.559183	-3.691812	-0.945750
C	0.395383	-2.609929	-2.778318
C	2.067505	-4.633696	-1.834425
C	0.911317	-3.551450	-3.661077
C	1.744809	-4.563524	-3.187996
H	1.804689	-3.749784	0.111887
H	-0.266779	-1.823947	-3.138646
H	2.715108	-5.424620	-1.468651
H	0.655697	-3.503151	-4.715046
H	2.140160	-5.303883	-3.876988
C	0.110974	-2.044211	1.363196
C	-0.596951	-3.221142	1.653307
C	0.696318	-1.317050	2.406414
C	-0.708431	-3.662649	2.966945
C	0.580701	-1.766319	3.718835
C	-0.123417	-2.934001	4.001288
H	-1.053877	-3.796183	0.849727
H	1.253458	-0.408540	2.191332
H	-1.252234	-4.577403	3.182763
H	1.045236	-1.202509	4.522234
H	-0.214088	-3.278492	5.026849
C	1.806504	2.224583	-0.771913
H	1.842418	2.354875	-1.862306
H	1.435059	3.174593	-0.378592
C	3.178328	1.913277	-0.239768
C	3.461344	2.065294	1.121970
C	4.188804	1.436838	-1.079302
C	4.720402	1.759385	1.623333

C	5.449374	1.132543	-0.573388
C	5.739771	1.292096	0.784993
H	2.686145	2.433591	1.792907
H	3.988274	1.314281	-2.142199
H	4.924037	1.890479	2.683665
H	6.224421	0.770544	-1.245076
C	7.105930	1.003062	1.322095
H	7.079136	0.753766	2.385974
H	7.586863	0.177451	0.790669
H	7.763692	1.873014	1.215081
Cr	-2.002620	-0.154364	-0.372068
H	-4.687859	-0.617967	-1.261079
H	-3.583923	0.103109	-0.000487
H	-2.791422	-1.689411	-2.386101
H	-2.577093	-2.774578	-0.940008
C	-3.948759	-1.112369	-0.621781
C	-2.870564	-1.788696	-1.302351
C	-3.155594	0.993270	1.121458
C	-4.532513	-1.742752	0.636792
C	-4.940071	-0.732617	1.706062
C	-3.755275	0.095882	2.199892
H	-2.234686	1.474337	1.467077
H	-3.842413	1.796563	0.826223
H	-5.387473	-2.369077	0.354723
H	-3.781611	-2.425443	1.062632
H	-5.714267	-0.061727	1.306507
H	-5.400658	-1.261358	2.546521
H	-4.058620	0.704383	3.062207
H	-2.980815	-0.589732	2.581089

L104 – Octene
Electronic Energy = -1973.962512
Enthalpy = -1973.190164
Free Energy = -1973.307373

N	0.811871	-1.251348	-0.562687
P	-0.398455	1.344044	-0.131069
C	1.488426	-2.497474	-0.403372
C	2.136335	-3.085143	-1.502970
C	1.556531	-3.072426	0.879824
C	2.862049	-4.260370	-1.295576
C	2.290408	-4.249653	1.042693
C	2.940675	-4.841678	-0.034682
H	3.368408	-4.719889	-2.140990
H	2.345623	-4.701637	2.030168
H	3.509489	-5.755276	0.109203
C	2.051085	-2.454067	-2.856727
H	2.285380	-1.384555	-2.815210
H	2.738476	-2.927146	-3.561565
H	1.044257	-2.527854	-3.285348
C	0.839701	-2.440878	2.031793
H	-0.251150	-2.516078	1.925369
H	1.106713	-2.915635	2.978525
H	1.055567	-1.368618	2.112649
Cr	1.945675	0.708615	-0.281281
C	3.904973	-0.192009	-0.444771
C	3.643518	-0.273325	1.061312
C	4.632361	0.507221	1.914726
C	4.665230	2.001253	1.623807
C	2.469905	2.601352	0.447730
C	3.299317	2.679111	1.721664
H	4.925648	0.144675	-0.614877
H	2.617013	0.049107	1.408170
H	5.627552	0.071491	1.768354
H	5.370575	2.467035	2.320059
H	1.548028	3.188931	0.573779

H	3.753127	-1.160204	-0.925701
H	3.614145	-1.334978	1.335785
H	4.380979	0.349761	2.971310
H	5.079624	2.178521	0.619803
H	3.017347	3.088783	-0.372792
H	2.744958	2.255866	2.576143
H	3.450945	3.736225	1.984146
C	2.027525	1.335758	-2.247952
H	1.741015	2.386043	-2.233555
H	1.426383	0.690224	-2.889126
C	3.397243	1.009329	-2.051865
H	4.078478	1.824576	-1.822425
H	3.844773	0.228888	-2.661075
C	-1.084349	2.688305	-1.122248
C	-1.232718	3.961547	-0.555739
C	-1.353739	2.499962	-2.484255
C	-1.657573	5.027277	-1.342731
C	-1.784792	3.569270	-3.261959
C	-1.935069	4.832482	-2.693552
H	-1.027882	4.116739	0.501213
H	-1.234024	1.514855	-2.928640
H	-1.776034	6.010063	-0.896956
H	-2.004071	3.415297	-4.314234
H	-2.269785	5.665560	-3.304196
C	-1.151350	1.489608	1.513777
C	-0.348450	1.240165	2.633291
C	-2.521952	1.731225	1.684701
C	-0.907016	1.222308	3.907958
C	-3.076600	1.709355	2.958835
C	-2.271076	1.452030	4.068252
H	0.720914	1.066137	2.500318
H	-3.150855	1.937366	0.820674
H	-0.279746	1.032746	4.773625
H	-4.138731	1.894890	3.088415
H	-2.708818	1.437536	5.061838
C	-1.313551	-2.502245	-0.919223
H	-1.197858	-2.839851	-1.957243
H	-0.849277	-3.285472	-0.309482
C	-2.771123	-2.345354	-0.581693
C	-3.172104	-2.055320	0.729879
C	-3.757590	-2.456842	-1.563410
C	-4.514462	-1.890602	1.043864
C	-5.103530	-2.297957	-1.243427
C	-5.507962	-2.015500	0.063594
H	-2.422213	-1.950826	1.514485
H	-3.469536	-2.676194	-2.589583
H	-4.801212	-1.666385	2.069319
H	-5.855298	-2.394448	-2.023322
C	-6.955823	-1.869709	0.413323
H	-7.125931	-1.041117	1.107218
H	-7.571488	-1.700144	-0.473209
H	-7.337635	-2.771613	0.904734
C	-0.478021	-1.253108	-0.751334
N	-1.144030	-0.059618	-0.817257
H	-2.156714	-0.127434	-0.860612

L105 – Hexene

Electronic Energy = -1590.531079
Enthalpy = -1590.872754
Free Energy = -1590.975401

Cr	1.262536	0.942044	0.225846
N	0.420919	-2.119067	-0.256368
C	-0.723658	-1.373620	-0.127292
N	-0.587985	-0.086713	0.068704
P	1.941930	-1.384158	0.173748

H	0.295000	-3.123407	-0.199851
C	-1.692277	0.799212	0.175246
C	-1.719418	1.639604	1.294285
C	-2.652065	0.931458	-0.824220
C	-2.715136	2.604439	1.436174
C	-3.662992	1.892795	-0.702473
C	-3.677673	2.715531	0.424533
H	-4.458606	3.468401	0.518123
C	-1.990622	-2.131981	-0.181047
C	-3.013213	-1.891487	0.746626
C	-2.147069	-3.149214	-1.133050
C	-4.168527	-2.661901	0.719794
C	-3.316429	-3.900460	-1.168235
C	-4.325789	-3.661075	-0.239465
H	-2.893968	-1.113399	1.494725
H	-1.362859	-3.329411	-1.864940
H	-4.949805	-2.481044	1.451289
H	-3.437326	-4.673960	-1.920176
H	-5.235731	-4.252879	-0.261095
C	2.468233	-2.415950	1.613814
C	3.942720	-2.197660	1.930012
H	4.597550	-2.477936	1.099500
H	4.231462	-2.807064	2.791211
H	4.148926	-1.153828	2.188638
C	3.055966	-1.814941	-1.233918
C	3.164578	-3.310593	-1.495060
H	3.537499	-3.865406	-0.628850
H	3.856179	-3.499060	-2.321630
H	2.197278	-3.735796	-1.785868
H	-0.956506	1.518233	2.065958
H	-2.612831	0.287230	-1.700116
C	-2.755276	3.506596	2.630050
H	-1.925450	3.313838	3.314545
H	-2.707672	4.560160	2.336161
H	-3.685352	3.384876	3.194770
C	-4.693902	2.039559	-1.778052
H	-5.430058	2.807089	-1.529106
H	-4.238039	2.315714	-2.734669
H	-5.233839	1.102403	-1.948383
C	2.970082	1.354282	1.319624
C	2.558417	2.616430	0.749864
C	3.396622	3.228767	-0.365520
C	2.577483	3.973837	-1.415897
C	0.553494	2.421656	-1.263952
C	1.618325	3.046243	-2.159732
H	3.903144	0.921372	0.955729
H	1.390791	2.560999	-0.024593
H	3.960139	2.421467	-0.857907
H	2.009456	4.783006	-0.934914
H	-0.195274	3.156504	-0.943674
H	2.795907	1.179953	2.382471
H	2.147999	3.348518	1.453024
H	4.146359	3.892421	0.081101
H	3.252328	4.458148	-2.128524
H	0.010739	1.621218	-1.782802
H	1.135128	3.590519	-2.981767
H	2.207960	2.251273	-2.641964
H	2.317491	-3.464111	1.315162
H	4.036444	-1.428128	-0.920104
C	1.573997	-2.106759	2.808568
H	1.678111	-1.061130	3.120647
H	0.515669	-2.290563	2.597213
H	1.849943	-2.732855	3.662169
C	2.603294	-1.042854	-2.467951
H	1.590612	-1.330882	-2.772166
H	2.606654	0.041110	-2.295905

H	3.269198	-1.241311	-3.312670

L105 – Octene
Electronic Energy = -1590.531079
Enthalpy = -1590.872754
Free Energy = -1590.975401

N	-0.498025	2.143852	0.064213
C	0.699246	1.470935	0.098225
N	0.681050	0.180355	0.303222
P	-2.003546	1.314089	0.267221
H	-0.442885	3.154240	0.101816
C	1.870657	-0.592596	0.235074
C	2.274681	-1.294010	1.374568
C	2.571389	-0.747205	-0.962779
C	3.383678	-2.142024	1.331961
C	3.683273	-1.592117	-1.029336
C	4.069042	-2.285412	0.121101
H	4.927114	-2.954078	0.074221
C	1.894799	2.319284	-0.119754
C	3.071144	2.138062	0.620554
C	1.839426	3.347027	-1.073637
C	4.163518	2.969164	0.407685
C	2.942006	4.164118	-1.294070
C	4.105032	3.977849	-0.552116
H	3.124235	1.357126	1.372356
H	0.938880	3.487158	-1.667742
H	5.065782	2.827509	0.994320
H	2.892683	4.944120	-2.047632
C	-2.777887	2.198202	1.694247
C	-4.214987	1.723998	1.879358
H	-4.829183	1.866698	0.984838
H	-4.690002	2.279628	2.693057
H	-4.248912	0.662130	2.147114
C	-2.985736	1.819029	-1.221060
C	-3.296696	3.308504	-1.283198
H	-3.887285	3.658189	-0.432291
H	-3.869181	3.532710	-2.188180
H	-2.378726	3.906677	-1.332984
Cr	-1.237808	-1.017388	0.357309
C	-0.307646	-2.948517	-0.160550
C	-0.590531	-2.315098	-1.529864
C	-1.547688	-3.104992	-2.413678
C	-2.913808	-3.377843	-1.799359
C	-3.201092	-1.682082	0.093127
C	-3.641067	-2.134684	-1.292352
H	-0.702673	-3.962477	-0.150914
H	-0.972983	-1.254899	-1.531212
H	-1.063374	-4.052865	-2.675944
H	-3.523267	-3.889760	-2.551776
H	-3.870019	-0.888468	0.457086
H	0.764827	-2.966768	0.023494
H	0.376851	-2.164976	-2.023368
H	-1.676210	-2.558044	-3.356984
H	-2.814255	-4.090546	-0.967205
H	-3.325181	-2.516739	0.800276
H	-3.528147	-1.321694	-2.028852
H	-4.719649	-2.349790	-1.276052
C	-1.227874	-1.527136	2.337681
H	-2.247727	-1.436761	2.708973
H	-0.480361	-0.934963	2.865323
C	-0.830876	-2.785294	1.787411
H	-1.591683	-3.559904	1.749777
H	0.158375	-3.160433	2.038404
H	2.248235	-0.203064	-1.848421
H	1.717030	-1.168087	2.300877

C	4.453486	-1.739938	-2.304702
H	5.389585	-1.171648	-2.268998
H	4.728000	-2.781534	-2.494257
H	3.888810	-1.376650	-3.167131
C	3.835066	-2.875388	2.557028
H	3.074622	-2.864403	3.342584
H	4.078494	-3.918895	2.336612
H	4.741849	-2.426681	2.977723
H	4.965677	4.617745	-0.721300
H	-2.782537	3.263821	1.422561
H	-3.924084	1.254626	-1.113990
C	-2.278315	1.350055	-2.486738
H	-1.328012	1.876223	-2.630115
H	-2.069537	0.274633	-2.474829
H	-2.899423	1.550829	-3.364387
C	-1.955663	2.019148	2.962744
H	-1.948497	0.974877	3.288653
H	-0.918089	2.343333	2.839833
H	-2.389235	2.612145	3.773447

New ligands designed from machine learning results. Labels match those in Figure 5 of main text

L9 – Hexene
Electronic Energy = -1046.1740602
Enthalpy = -1045.813641
Free Energy = -1045.879606

N	0.066400	-1.744685	-0.949511
C	0.812243	-0.775279	-0.393715
C	1.675806	1.304972	1.269108
Cr	-1.961167	-1.756317	-0.565633
H	-4.512315	-1.881394	-1.893135
H	-3.574376	-1.873258	-0.311912
H	-2.138685	-0.092097	-2.597612
H	-2.406969	-1.802737	-3.172507
C	-3.758172	-1.153462	-1.579436
C	-2.560192	-1.073573	-2.377332
C	-3.309448	-1.966597	1.095106
C	-4.321333	0.104815	-0.934120
C	-4.928618	-0.126194	0.449826
C	-3.894759	-0.608758	1.470226
H	-4.034630	-2.776823	1.227172
H	-2.417805	-2.232012	1.689356
H	-3.513947	0.849320	-0.849584
H	-5.066967	0.544315	-1.607898
H	-5.387332	0.801067	0.805162
H	-5.743508	-0.859996	0.376401
H	-3.089687	0.136923	1.542258
H	-4.346467	-0.661393	2.468369
C	2.830903	0.311655	1.328989
C	3.217375	-0.251385	-0.027406
C	0.938705	-2.646925	-1.509119
C	2.220862	-2.237720	-1.268739
N	2.123958	-1.059913	-0.567546
H	1.985197	2.204256	0.724369
H	1.418054	1.628848	2.280709
H	3.705307	0.813713	1.754121
H	2.593741	-0.519206	2.003216
H	4.094405	-0.897604	0.042968
H	3.450212	0.549770	-0.738706
H	3.176541	-2.673169	-1.516198
H	0.593966	-3.524427	-2.034462
P	0.110289	0.675177	0.456433
C	-0.011906	1.845989	-0.964148

H	-0.293966	2.829154	-0.576692
H	0.924327	1.943817	-1.521266
H	-0.799150	1.526781	-1.651884

L9 – Octene

Electronic Energy = -1083.0270184
Enthalpy = -1082.683229
Free Energy = -1082.747039

N	-0.673366	-3.089038	-0.621149
C	0.561944	-2.678855	-0.957317
C	2.765044	-1.301146	-1.407036
C	3.294628	-2.528666	-1.848137
C	2.593416	-3.701718	-1.854853
C	-0.720794	-4.432643	-0.871769
C	0.472937	-4.876330	-1.369528
N	1.293925	-3.769667	-1.426960
H	3.017895	-4.639204	-2.191867
H	4.319058	-2.565829	-2.203709
H	3.417408	-0.431974	-1.440043
Cr	-2.138838	-1.693695	0.238561
C	-3.962783	-2.473080	-0.575868
C	-3.598255	-1.427479	-1.648401
C	-4.569768	-0.262053	-1.758432
C	-4.670032	0.614548	-0.516615
C	-2.633120	0.158512	0.913372
C	-3.313595	1.127961	-0.029187
H	-5.044976	-2.462411	-0.462148
H	-2.560980	-1.003189	-1.594305
H	-5.556899	-0.664839	-2.014771
H	-5.338928	1.450393	-0.744166
H	-1.603883	0.477899	1.169481
H	-3.650721	-3.476119	-0.881765
H	-3.537152	-1.975921	-2.595126
H	-4.262274	0.357248	-2.609734
H	-5.154982	0.057190	0.298873
H	-3.192924	0.075988	1.854890
H	-2.670531	1.345881	-0.896047
H	-3.452738	2.094931	0.474390
C	-2.551696	-2.656343	1.972201
H	-2.352272	-1.935248	2.764062
H	-2.027737	-3.607325	2.063199
C	-3.860199	-2.662619	1.384997
H	-4.547938	-1.877403	1.692394
H	-4.347729	-3.626035	1.259607
H	-1.610844	-5.014353	-0.675026
H	0.815338	-5.850076	-1.681306
P	1.182385	-1.028886	-0.809231

L10 – Hexene

Electronic Energy = -1008.0705732
Enthalpy = -1007.718705
Free Energy = -1007.787541

N	0.387952	-1.664082	0.621102
C	1.353173	-0.813686	0.241374
C	3.791102	-0.894145	-0.323802
C	1.027807	1.527290	-1.496170
C	0.952434	-2.906381	0.670562
C	2.274760	-2.806069	0.314591
N	2.515815	-1.481731	0.044005
H	0.593669	0.860697	-2.244162
H	0.528034	2.496039	-1.585678
H	4.338241	-1.580983	-0.969040
H	4.388751	-0.683071	0.566084
H	0.389793	-3.785785	0.946237
H	3.053446	-3.548275	0.223758

P	0.733844	0.877772	0.180818
C	1.828555	1.891670	1.229718
H	1.459408	2.920523	1.231561
H	1.816896	1.529028	2.259291
H	2.858395	1.900061	0.862563
Cr	-1.364717	-0.420618	0.804025
H	-4.087334	-0.511949	-0.062291
H	-2.840866	-0.999100	1.184454
H	-2.363934	1.991098	0.167075
H	-2.430771	0.849907	-1.260218
C	-3.448276	0.140355	0.541008
C	-2.520049	0.969310	-0.179499
C	-2.233975	-1.730361	2.317292
C	-4.115206	0.690255	1.795252
C	-4.261485	-0.325006	2.926278
C	-2.914115	-0.880293	3.384421
H	-2.814909	-2.632516	2.090645
H	-1.234439	-2.061487	2.622173
H	-3.519353	1.540083	2.159072
H	-5.094530	1.102029	1.523310
H	-4.776974	0.145883	3.768843
H	-4.903987	-1.155740	2.601446
H	-2.258811	-0.037104	3.660003
H	-3.038156	-1.466092	4.304462
H	2.090618	1.671021	-1.710004
H	3.614282	0.032480	-0.871559

L10 – Octene

Electronic Energy = -1086.6804149
Enthalpy = -1086.267292
Free Energy = -1086.341298

N	0.365582	-1.912445	0.093040
C	1.387904	-1.058237	0.239486
C	3.895335	-1.159596	0.381861
C	1.598499	1.656003	-0.844352
C	0.914823	-3.153402	-0.048745
C	2.282729	-3.053323	0.017786
N	2.571455	-1.725071	0.199800
H	1.211639	2.675809	-0.768874
H	2.688527	1.700012	-0.771276
H	4.600052	-1.646415	-0.292272
H	4.232312	-1.293282	1.412576
Cr	-1.425386	-0.524541	0.464281
C	-2.827294	-2.120315	0.083564
C	-2.734815	-1.456194	-1.296405
C	-4.032904	-0.830636	-1.785569
C	-4.590183	0.264766	-0.886130
C	-2.689639	1.101126	0.592181
C	-3.595639	1.388153	-0.592570
H	-3.868872	-2.356154	0.292932
H	-1.929112	-0.678507	-1.420090
H	-4.772692	-1.631238	-1.902379
H	-5.490652	0.666517	-1.362437
H	-2.015976	1.948751	0.786508
H	-2.231187	-3.033203	0.120082
H	-2.369462	-2.215940	-1.996696
H	-3.863696	-0.421996	-2.789481
H	-4.927986	-0.169986	0.066889
H	-3.298647	0.971973	1.499027
H	-3.001903	1.594527	-1.497767
H	-4.154910	2.316120	-0.404199
C	-1.514667	-0.896012	2.480011
H	-1.662527	0.071735	2.956337
H	-0.651150	-1.467556	2.818746
C	-2.665701	-1.622334	2.056799

H	-3.633122	-1.138587	2.163474
H	-2.692567	-2.691943	2.242951
H	0.313449	-4.038778	-0.195023
H	3.065149	-3.794201	-0.050345
P	0.844019	0.647741	0.475162
C	1.620741	1.270794	2.001106
H	1.213613	2.26202	2.218588
H	1.377099	0.619901	2.843693
H	2.707183	1.359261	1.915713
H	3.869755	-0.09523	0.147946
H	1.320434	1.263801	-1.82481

L11 – Hexene
Electronic Energy = -1332.7242978
Enthalpy = -1332.369122
Free Energy = -1332.437500

C	1.315896	-1.358009	-0.761598
C	3.861153	-0.960293	0.126895
C	3.698410	0.443891	-0.455325
C	2.351579	1.122612	-0.209899
C	0.808921	-3.214900	0.397332
C	2.138893	-3.460718	0.259943
H	2.395265	2.173284	-0.515593
H	2.114580	1.124075	0.859833
H	4.465484	1.067643	0.018397
H	3.945460	0.445732	-1.523909
H	4.907864	-1.268282	0.083655
H	3.544984	-0.994300	1.174057
H	0.084854	-3.861110	0.882654
H	2.618644	-4.374449	0.589111
P	0.901462	0.369295	-1.089048
C	1.237716	0.667077	-2.856754
H	1.021824	1.712425	-3.093156
H	2.273756	0.450447	-3.131212
H	0.578579	0.043511	-3.464714
Cr	-1.334626	-0.674700	-0.259103
H	-4.024604	-0.835684	-1.202976
H	-2.841800	-1.107492	0.187391
H	-2.191642	1.602666	-1.358878
H	-2.272494	0.224331	-2.560514
H	-3.388764	-0.095202	-0.708267
C	-2.395287	0.544749	-1.525036
C	-2.300176	-1.608459	1.458984
C	-4.080239	0.703588	0.387978
C	-4.310620	-0.068314	1.685255
C	-3.003572	-0.555458	2.307374
H	-2.881559	-2.535995	1.396107
H	-1.317476	-1.872724	1.868039
H	-3.466629	1.589277	0.607745
H	-5.031517	1.084338	-0.002523
H	-4.843383	0.571918	2.394913
H	-4.968112	-0.928898	1.497112
H	-2.334782	0.309727	2.447343
H	-3.185383	-0.951720	3.314549
P	2.868355	-2.242767	-0.829291
N	0.354033	-2.004854	-0.129234

L11 – Octene
Electronic Energy = -1411.3356189
Enthalpy = -1410.919255
Free Energy = -1410.992613

6	1.446125	-1.344197	0.351187
6	3.290454	-1.480998	2.377265
6	3.271980	0.047314	2.339195

6	1.895687	0.690126	2.177734
6	0.749723	-3.468636	0.337881
6	2.019008	-3.721925	0.757920
1	1.967057	1.775130	2.309962
1	1.214010	0.332702	2.957843
1	3.682976	0.392951	3.294719
1	3.965292	0.419527	1.574826
1	4.267156	-1.840476	2.708608
1	2.539362	-1.869834	3.072502
24	-1.308994	-0.576542	0.414283
6	-2.785784	-2.100825	-0.013131
6	-2.611068	-1.431071	-1.383709
6	-3.858111	-0.744123	-1.920704
6	-4.399612	0.372176	-1.03784
6	-2.526060	1.074636	0.540123
6	-3.360461	1.433256	-0.676285
1	-3.846671	-2.262516	0.168362
1	-1.769680	-0.686934	-1.47152
1	-4.628417	-1.509038	-2.072751
1	-5.248775	0.830207	-1.555435
1	-1.816633	1.877851	0.787024
1	-2.259682	-3.055451	0.017552
1	-2.251903	-2.201478	-2.074917
1	-3.627080	-0.340492	-2.91417
1	-4.811748	-0.052239	-0.110042
1	-3.179355	0.945551	1.415072
1	-2.716931	1.627716	-1.549389
1	-3.877712	2.385522	-0.48996
6	-1.446085	-0.983172	2.417947
1	-1.575100	-0.022919	2.914584
1	-0.611473	-1.591051	2.769033
6	-2.615734	-1.663071	1.9627
1	-3.566635	-1.149578	2.076147
1	-2.680470	-2.734330	2.130294
1	-0.011352	-4.218211	0.144198
1	2.420467	-4.718438	0.896586
15	1.050570	0.407360	0.555006
6	2.091347	1.306625	-0.64304
1	1.950279	2.382224	-0.510476
1	3.152224	1.071802	-0.519075
1	1.794912	1.051081	-1.662365
15	2.975995	-2.216066	0.67749
7	0.404558	-2.128444	0.158904

L12 – Hexene

Electronic Energy = -1336.1255261
Enthalpy = -1335.679716
Free Energy = -1335.760544

P	-1.62708	0.33119	0.03769
Cr	0.66472	-0.32809	-0.38846
H	2.58831	-2.44737	-0.26405
H	2.23745	-0.68912	-0.62086
H	0.52290	-1.73185	1.86601
H	0.25199	-2.81539	0.41644
C	2.13457	-1.70087	0.39452
C	0.78627	-1.96141	0.83286
C	2.40933	0.69602	-1.10885
C	3.10511	-1.02486	1.35485
C	4.04518	-0.01652	0.69748
C	3.28840	1.14359	0.05109
H	3.00166	0.36368	-1.96885
H	1.73842	1.49256	-1.47084
H	2.52160	-0.51232	2.13460
H	3.68063	-1.80130	1.87266
H	4.74421	0.36832	1.44590

H	4.65848	-0.52064	-0.06254
H	2.67195	1.63778	0.81874
H	3.99385	1.91046	-0.29342
N	-1.09680	1.30888	-1.34161
C	-0.70196	0.69419	-2.54043
C	-0.75738	2.64642	-1.40482
C	-0.15764	1.66493	-3.35028
H	-0.99452	-0.32923	-2.74337
C	-0.18298	2.88511	-2.63319
H	-0.95031	3.30066	-0.56666
H	0.21060	1.51044	-4.35468
H	0.17001	3.84589	-2.98078
C	-3.16358	-0.42342	-0.51920
C	-3.48898	-1.68047	0.00781
C	-4.01625	0.19727	-1.44205
C	-4.67310	-2.30283	-0.37233
C	-2.81732	-2.16862	0.71091
C	-5.19268	-0.43906	-1.82268
H	-3.75365	1.16494	-1.86335
C	-5.52143	-1.68363	-1.28720
H	-4.92731	-3.27531	0.03718
H	-5.85376	0.03679	-2.54031
H	-6.44022	-2.17614	-1.59044
C	-1.99443	1.56343	1.29726
C	-0.94386	1.96661	2.13424
C	-3.26738	2.12726	1.44911
C	-1.15772	2.94518	3.09723
H	0.04013	1.50707	2.02935
C	-3.47555	3.10061	2.42015
H	-4.08764	1.80273	0.81375
C	-2.42404	3.51066	3.23794
H	-0.34351	3.25932	3.74248
H	-4.46122	3.53918	2.53977
H	-2.59396	4.26941	3.99573

L12 – Octene

Electronic Energy = -1414.7411282
Enthalpy = -1414.234426
Free Energy = -1414.323263

P	1.628223	0.177828	0.251712
Cr	-0.771531	-0.363132	0.632085
C	-2.441114	-1.628775	0.289109
C	-2.369171	-0.894109	-1.052165
C	-3.543184	0.029792	-1.334954
C	-3.722230	1.154581	-0.323997
C	-1.492195	1.541878	0.865777
C	-2.483293	2.036837	-0.168578
H	-3.481412	-1.765075	0.576748
H	-1.418013	-0.310878	-1.232751
H	-4.451030	-0.582943	-1.378956
H	-4.580117	1.758533	-0.635534
H	-0.602946	2.184844	0.919424
H	-1.949741	-2.606392	0.235026
H	-2.262850	-1.657628	-1.831578
H	-3.415858	0.460304	-2.335489
H	-3.991685	0.738273	0.658342
H	-1.956008	1.533576	1.862602
H	-1.999161	2.160745	-1.149863
H	-2.798195	3.050442	0.118705
C	-0.761587	-0.836496	2.627123
H	-0.621541	0.115774	3.134964
H	-0.028269	-1.606691	2.867984
C	-2.081695	-1.244281	2.297596
H	-2.898409	-0.547606	2.475176
H	-2.356970	-2.284326	2.440521

N	1.901782	-1.316668	-0.629309
C	1.916626	-1.461992	-2.004076
C	1.510844	-2.530729	-0.066922
C	1.591886	-2.763205	-2.305598
H	2.167924	-0.624944	-2.639663
C	1.336669	-3.438859	-1.084715
H	1.495840	-2.649876	1.009264
H	1.572592	-3.191275	-3.298036
H	1.094448	-4.485584	-0.961496
C	2.178174	1.441360	-0.914081
C	1.209873	2.060464	-1.715121
C	3.528697	1.781334	-1.061998
C	1.588856	3.000223	-2.667091
H	0.158923	1.800627	-1.588479
C	3.901099	2.722832	-2.014750
H	4.281480	1.312455	-0.433114
C	2.934507	3.329548	-2.815569
H	0.836927	3.478720	-3.286872
H	4.947939	2.985590	-2.131497
H	3.231937	4.066741	-3.555129
C	2.842073	0.103437	1.588312
C	2.573016	0.841344	2.748574
C	4.022388	-0.644773	1.492527
C	3.482890	0.839206	3.799976
H	1.652521	1.417584	2.825876
C	4.923460	-0.647148	2.552547
H	4.226777	-1.226177	0.596747
C	4.655591	0.093336	3.702333
H	3.273066	1.413191	4.697188
H	5.837578	-1.228480	2.480037
H	5.362435	0.086160	4.526616

L13 – Hexene

Electronic Energy = -1337.3404452
Enthalpy = -1336.870529
Free Energy = -1336.948642

P	0.693578	0.943924	-0.307333
C	0.614865	3.634969	-0.414378
C	2.861660	2.685630	-0.289787
H	3.108619	2.926765	0.752536
N	1.436129	2.433217	-0.462247
H	3.454911	1.823789	-0.595462
H	0.701852	4.152246	0.550265
C	1.252670	-0.174572	1.135448
C	1.531968	-0.457978	-1.283919
C	0.398171	-1.315342	0.646251
C	2.693609	-0.452373	0.804366
H	1.036969	0.177619	2.144877
C	0.554122	-1.478394	-0.749027
C	2.853658	-0.624852	-0.580549
H	1.562317	-0.357983	-2.369492
C	4.104925	-0.881282	-1.123383
C	5.205629	-0.948079	-0.264297
C	5.048421	-0.768615	1.108063
C	3.786405	-0.523271	1.655839
H	4.230557	-1.014554	-2.194578
H	6.193658	-1.137464	-0.672790
H	5.915092	-0.817813	1.760353
H	3.666399	-0.383274	2.726974
C	-0.537088	-2.077273	1.343948
C	-1.287486	-3.025565	0.647686
C	-1.127569	-3.191298	-0.730382
C	-0.216295	-2.409885	-1.442333
H	-0.668291	-1.944669	2.415308
H	-2.004508	-3.641513	1.182960

H	-1.719242	-3.936878	-1.253252
H	-0.098439	-2.536099	-2.515488
H	0.922309	4.327141	-1.205714
H	-0.440386	3.384200	-0.574090
H	3.148399	3.537069	-0.914834
Cr	-1.756456	0.825947	-0.420463
H	-3.751046	2.273972	1.082174
H	-3.348325	1.187484	-0.306217
H	-1.399337	0.684738	2.186143
H	-1.379909	2.449834	1.709737
C	-3.170540	1.347081	1.105474
C	-1.792035	1.458747	1.523841
C	-3.507342	0.387485	-1.532402
C	-3.964352	0.101774	1.486427
C	-4.934006	-0.380888	0.407495
C	-4.215153	-0.792578	-0.879926
H	-4.210073	1.108444	-1.962363
H	-2.807428	0.091788	-2.338889
H	-3.252481	-0.707635	1.711889
H	-4.502499	0.302407	2.420624
H	-5.510252	-1.227777	0.791015
H	-5.664725	0.408970	0.184289
H	-3.485852	-1.582052	-0.641892
H	-4.925336	-1.243471	-1.583988

L13 – Octene

Electronic Energy = -1415.9543661
Enthalpy = -1415.422850
Free Energy = -1415.506158

P	-0.682644	-0.924919	0.17466
C	-2.614745	-2.786433	0.875825
C	-0.701853	-3.522743	-0.444707
H	-1.313668	-3.694709	-1.341126
N	-1.270698	-2.479882	0.402421
H	0.305853	-3.249041	-0.769958
H	-3.367106	-2.763550	0.075462
Cr	1.637340	-0.113202	0.455124
C	3.237321	1.301895	0.206925
C	3.062707	0.787748	-1.227986
C	4.228436	-0.001238	-1.80455
C	4.590063	-1.276105	-1.055215
C	2.630879	-1.905001	0.428722
C	3.409923	-2.221368	-0.830103
H	4.297390	1.419805	0.42321
H	2.119323	0.199236	-1.416857
H	5.098525	0.664018	-1.848198
H	5.381881	-1.783256	-1.615368
H	1.845884	-2.641926	0.644152
H	2.730113	2.264578	0.327432
H	2.845346	1.666944	-1.846874
H	3.986004	-0.251991	-2.8445
H	5.031304	-1.024250	-0.079562
H	3.306555	-1.890633	1.294754
H	2.755183	-2.218631	-1.716812
H	3.786211	-3.252481	-0.759935
C	1.781586	0.031091	2.492795
H	1.801496	-0.990411	2.86698
H	0.997744	0.667049	2.903997
C	3.015284	0.649240	2.128697
H	3.918310	0.046136	2.181379
H	3.170842	1.685457	2.415586
C	-1.694793	0.330829	1.137906
C	-1.417009	0.084443	-1.280551
C	-0.911032	1.506320	0.578673
C	-3.044062	0.293163	0.454914

H	-1.689050	0.241903	2.225457
C	-0.756892	1.359420	-0.818058
C	-2.879747	0.133403	-0.930274
H	-1.161887	-0.237789	-2.291108
C	-3.983527	0.043634	-1.766493
C	-5.259736	0.112673	-1.200918
C	-5.421117	0.280671	0.172228
C	-4.309740	0.377126	1.014946
H	-3.860131	-0.082216	-2.838968
H	-6.134155	0.034920	-1.839939
H	-6.419952	0.331381	0.594726
H	-4.438256	0.499317	2.087454
C	-0.376481	2.612276	1.237426
C	0.300950	3.577319	0.490383
C	0.461288	3.428524	-0.889447
C	-0.056667	2.315033	-1.552352
H	-0.501550	2.730246	2.310715
H	0.705024	4.454380	0.987036
H	0.988286	4.192215	-1.454187
H	0.065560	2.203492	-2.626880
H	-2.602997	-3.792177	1.307736
H	-2.918710	-2.088304	1.656548
H	-0.637195	-4.461426	0.115100

L14 – Hexene

Electronic Energy = -1113.5512858
Enthalpy = -1113.029954
Free Energy = -1113.109398

P	-1.194850	0.182441	-0.219567
C	0.114152	1.133905	1.993839
C	-0.904738	-1.007658	2.387236
H	-1.742903	-0.565121	2.938610
N	-0.401168	-0.093982	1.353184
H	-1.225444	-1.954717	1.959815
H	-0.664507	1.675494	2.544762
C	-2.574982	1.470300	-0.012340
C	-1.859337	-1.500400	-0.778792
H	0.900731	0.852506	2.701483
H	0.540837	1.814613	1.244459
H	-0.093189	-1.213341	3.091528
C	-3.380686	1.247975	1.265590
H	-2.776356	1.371051	2.168933
H	-4.181928	1.994310	1.315025
H	-3.853349	0.263075	1.303521
C	-1.920323	2.856358	0.009205
H	-1.287617	3.025896	-0.867925
H	-2.708883	3.616862	-0.003025
H	-1.321460	3.037437	0.903672
C	-3.498925	1.414903	-1.230586
H	-2.953870	1.506058	-2.175466
H	-4.106840	0.507891	-1.263344
H	-4.190751	2.262354	-1.174067
C	-3.129361	-2.007885	-0.098035
H	-3.398994	-2.977823	-0.531146
H	-3.021509	-2.156013	0.979190
H	-3.979674	-1.341124	-0.263128
C	-2.112402	-1.363905	-2.290693
H	-1.256252	-0.924726	-2.815251
H	-2.267668	-2.365534	-2.705689
H	-2.999582	-0.777747	-2.531499
C	-0.723842	-2.524730	-0.633311
H	-1.074751	-3.490686	-1.012706
H	0.148920	-2.258051	-1.247335
H	-0.383655	-2.689145	0.391687
Cr	1.264597	-0.318278	-0.033049

H	3.700205	-1.857561	-0.339318
H	2.643081	-0.490589	-0.900135
H	2.421071	-0.944197	2.268195
H	2.012433	-2.473276	1.350597
C	3.272292	-1.052564	0.265770
C	2.341449	-1.435082	1.296189
C	2.204431	0.624873	-1.764641
C	4.218100	0.112983	0.526611
C	4.476777	0.998850	-0.690586
C	3.201529	1.647496	-1.229372
H	2.609469	0.095098	-2.635019
H	1.258082	1.075481	-2.083220
H	3.789870	0.733386	1.330010
H	5.163464	-0.277204	0.922764
H	5.200999	1.774301	-0.423177
H	4.946462	0.405807	-1.487832
H	2.737346	2.239628	-0.423015
H	3.452013	2.373038	-2.014060

L14 – Octene

Electronic Energy = -1192.1638278
Enthalpy = -1191.580161
Free Energy = -1191.662570

P	-1.274260	0.103034	0.189836
C	-2.966420	-0.470888	2.359361
C	-0.635227	-1.120660	2.510774
H	-0.608425	-2.182881	2.212912
N	-1.627726	-0.328323	1.804154
H	0.368789	-0.684811	2.392134
H	-3.288801	-1.521115	2.411135
Cr	1.156857	-0.701724	0.046515
C	2.998743	-1.047851	1.117881
C	2.839649	0.455403	1.315803
C	3.886111	1.311095	0.616916
C	3.959391	1.120789	-0.892372
C	1.729076	0.169917	-1.714896
C	2.635470	1.379807	-1.612935
H	4.040585	-1.291761	0.920549
H	1.826731	0.860708	1.036914
H	4.860273	1.091289	1.068881
H	4.734193	1.789834	-1.279353
H	0.784600	0.406520	-2.222765
H	2.653781	-1.613000	1.989974
H	2.824051	0.652088	2.395074
H	3.677546	2.365303	0.838294
H	4.302524	0.101789	-1.126365
H	2.218843	-0.631421	-2.286305
H	2.112955	2.220465	-1.129965
H	2.848967	1.732119	-2.6327
C	1.197051	-2.635057	-0.690321
H	0.927326	-2.542841	-1.741105
H	0.578357	-3.316378	-0.105462
C	2.559728	-2.509599	-0.320897
H	3.279979	-2.200120	-1.074547
H	2.965545	-3.191043	0.419837
C	-1.542041	1.965610	0.123321
C	-2.432568	-0.811999	-0.99453
H	-2.992750	-0.063785	3.377702
H	-3.696581	0.078328	1.76504
H	-0.840446	-1.089159	3.586152
C	-2.857124	2.418380	0.757782
H	-2.881893	2.197041	1.828319
H	-2.943079	3.506211	0.653149
H	-3.741765	1.979958	0.289817
C	-0.392724	2.572017	0.932935

H	0.569748	2.445461	0.423502
H	-0.552737	3.649104	1.053925
H	-0.323618	2.135237	1.936274
C	-1.439864	2.456798	-1.319863
H	-0.519441	2.115054	-1.807384
H	-2.288147	2.146696	-1.936345
H	-1.421051	3.552578	-1.327421
C	-3.848680	-0.253158	-1.121517
H	-4.419289	-0.894996	-1.803096
H	-4.390536	-0.239936	-0.171952
H	-3.870036	0.755599	-1.542257
C	-1.769874	-0.816914	-2.376156
H	-0.784409	-1.292786	-2.350126
H	-2.393579	-1.389325	-3.072280
H	-1.651314	0.185284	-2.797864
C	-2.501207	-2.254132	-0.486627
H	-3.027681	-2.872377	-1.222241
H	-1.505377	-2.689269	-0.352505
H	-3.042874	-2.339864	0.459150

L15 – Hexene
Electronic Energy = -1303.0765875
Enthalpy = -1302.529644
Free Energy = -1302.612328

P	-0.752798	-1.322419	0.951323
C	-1.156346	-2.221788	2.541106
C	-1.568595	0.357381	0.743284
C	-2.603463	-2.698993	2.643137
H	-2.843030	-3.442699	1.879452
H	-2.740073	-3.181930	3.617192
H	-3.330673	-1.885055	2.583941
C	-0.228817	-3.441533	2.547595
H	0.827772	-3.154367	2.541990
H	-0.408763	-4.030990	3.452961
H	-0.412709	-4.096141	1.688579
C	-0.822997	-1.301865	3.716230
H	0.195424	-0.903949	3.664363
H	-1.520870	-0.462424	3.795046
H	-0.900228	-1.873703	4.647092
C	-3.012378	0.442378	1.225213
H	-3.412078	1.436246	0.993838
H	-3.661845	-0.286599	0.732365
H	-3.093947	0.305981	2.307472
C	-0.710942	1.390023	1.482390
H	0.306158	1.443675	1.072837
H	-1.161514	2.380807	1.359316
H	-0.631488	1.199344	2.556522
C	-1.482614	0.647911	-0.759698
H	-1.762232	1.690367	-0.945448
H	-0.456281	0.516879	-1.140661
H	-2.145767	0.008452	-1.349609
Cr	1.516106	-1.042305	0.008510
H	4.199584	-0.769224	0.873940
H	2.960944	-0.432033	-0.454771
H	1.760586	0.160364	2.434371
H	2.471816	-1.523836	2.434934
C	3.284163	-0.171232	0.924274
C	2.290109	-0.608104	1.871323
C	2.396623	-0.137736	-1.775001
C	3.495540	1.322907	0.714867
C	3.763674	1.730576	-0.731372
C	2.601078	1.367376	-1.652723
H	3.222055	-0.611709	-2.319720
H	1.470037	-0.384901	-2.312577
H	2.599608	1.851979	1.072193

H	4.317260	1.650842	1.362264
H	3.949648	2.807720	-0.775516
H	4.682525	1.247367	-1.092583
H	1.682024	1.835205	-1.263877
H	2.754040	1.800550	-2.648930
N	-1.477757	-2.298681	-0.300692
C	-0.723122	-2.759198	-1.357221
C	-2.813809	-2.582175	-0.614640
C	-1.511984	-3.337415	-2.310500
C	-2.847210	-3.218464	-1.823018
H	-3.604977	-2.308373	0.064313
H	-1.187913	-3.795427	-3.232864
H	-3.737798	-3.576752	-2.319447
O	0.635744	-2.564002	-1.281361
C	1.373030	-3.166098	-2.363506
H	2.427153	-2.994849	-2.148137
H	1.165840	-4.238627	-2.388761
H	1.099130	-2.702736	-3.315556

L15 – Octene

Electronic Energy = -1381.687985
Enthalpy = -1381.079403
Free Energy = -1381.166441

P	-1.187201	0.205905	0.242748
Cr	1.221721	-0.653194	0.256662
C	3.210745	-0.800741	1.154147
C	2.908347	0.687414	1.311422
C	3.826335	1.615549	0.527679
C	3.886231	1.350583	-0.970520
C	1.726746	0.125624	-1.588362
C	2.531081	1.411729	-1.671452
H	4.232289	-0.931229	0.801790
H	1.850688	0.993281	1.081786
H	4.831384	1.534107	0.957707
H	4.570777	2.081504	-1.413055
H	0.773214	0.224285	-2.125229
H	3.089062	-1.323141	2.103970
H	2.933994	0.916898	2.383182
H	3.504593	2.650391	0.701212
H	4.342492	0.367075	-1.159894
H	2.278168	-0.678908	-2.096686
H	1.958877	2.266174	-1.278245
H	2.695460	1.651783	-2.732200
C	1.363206	-2.595103	-0.415152
H	1.083596	-2.575596	-1.466653
H	0.786682	-3.277946	0.209016
C	2.730417	-2.375615	-0.084030
H	3.408878	-2.112740	-0.891249
H	3.190715	-3.002388	0.675785
C	-1.438172	2.059550	0.036042
C	-2.384631	-0.838397	-0.770367
C	-2.748208	2.618867	0.590999
H	-2.776550	2.579788	1.682442
H	-2.811631	3.675742	0.308575
H	-3.640446	2.128423	0.196677
C	-0.282685	2.724790	0.788516
H	0.679546	2.529083	0.304879
H	-0.428664	3.810410	0.789780
H	-0.228440	2.401845	1.834776
C	-1.328161	2.381931	-1.455926
H	-0.427320	1.959099	-1.914152
H	-2.200069	2.035011	-2.018098
H	-1.274809	3.468836	-1.580857
C	-3.800014	-0.279838	-0.874160
H	-4.421813	-0.995159	-1.424723

H	-4.266675	-0.139416	0.105173
H	-3.837372	0.665583	-1.422785
C	-1.783919	-0.999545	-2.169796
H	-0.799472	-1.477178	-2.137091
H	-2.440552	-1.640098	-2.768429
H	-1.683471	-0.050610	-2.704587
C	-2.421360	-2.206636	-0.082540
H	-2.971744	-2.908924	-0.717586
H	-1.416222	-2.620284	0.064864
H	-2.925200	-2.167250	0.887928
N	-1.639290	-0.117551	1.896222
C	-0.894488	-0.947535	2.711697
C	-2.874695	0.060417	2.536991
C	-1.593158	-1.272560	3.840900
C	-2.854513	-0.621789	3.719343
H	-3.639215	0.671532	2.088037
H	-1.248234	-1.889207	4.657379
H	-3.657069	-0.648463	4.442752
O	0.343846	-1.346218	2.273635
C	0.814562	-2.524163	2.952490
H	1.682126	-2.887875	2.402633
H	1.102604	-2.279584	3.978599
H	0.031615	-3.288329	2.955550