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Data Article

# Supporting plots and tables on vapour-liquid equilibrium prediction for synthesis gas conversion using artificial neural networks



# Precious Chukwuweike Eze, Cornelius Mduduzi Masuku\*

Department of Civil and Chemical Engineering, University of South Africa, Private Bag X6, Florida, 1710, South Africa

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## ABSTRACT

This article contains data on vapor-liquid equilibrium modeling of 1533 gas-liquid solubilities divided over sixty binary systems viz. carbon monoxide, carbon dioxide, hydrogen, water, ethane, propane, pentane, hexane, methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, and 1-hexanol in the solvents phenanthrene, 1-hexadecanol, octacosane, hexadecane and tetraethylene glycol at pressures up to 5.5 MPa and temperatures from 293 to 553 K using literature data. The solvents are considered to be potentially significant in the conversion of synthesis gas through gas-slurry processes. Artificial neural networks limited to one hidden layer and up to five neurons in the hidden layer were used to predict the binary plots.

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# Specifications table

Chemical Engineering Subject area More specific subject area Thermodynamic Phase Equilibria Type of data Tables, and Figures How data was acquired Generated through a code on MATLAB<sup>®</sup>

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\* Corresponding author.

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E-mail address: masukcm@unisa.ac.za (C.M. Masuku).

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Data format	Filtered
Experimental factors	Feature scaling
Experimental features	Code was implemented on MATLAB <sup>®</sup>
Data source location	Input experimental data was obtained from Breman et al. (1994).
Data accessibility	Source data is available on Journal of Chemical & Engineering Data:
	https://pubs.acs.org/doi/abs/10.1021/je00016a004
Related research article	P.C. Eze, C.M. Masuku, Vapour–Liquid Equilibrium Prediction for
	Synthesis Gas Conversion using Artificial Neural Networks, SAJCE
	(2018) in press.

# Value of the data

- This data could be used by the broader scientific community as it shows the training and testing of artificial neural networks for a number of binary systems.
- Different training algorithms could be used and compared with the performance described here.
- Other computational methods and techniques could be used and compared with the data presented here.

#### 1. Data

The data presented here is generated in preparation of a manuscript on vapour–liquid equilibrium (VLE) prediction for synthesis gas conversion using artificial neural networks (ANN) [1]. The experimental VLE data used in this study was obtained from Breman et al. [2]. Phase equilibrium modeling is a crucial element in describing the behavior of the Fischer–Tropsch (FT) reaction [3–12]. The FT reaction produces a range of hydrocarbons from light olefins and paraffins to heavy wax. Since we are comparing too many binaries to easily visualize, data for each binary is presented here. Then the summary of the overall results is published on the related paper [1]. The tables and figures presented here are unique; there is no duplication.

#### 2. Experimental design, materials, and methods

An artificial neural network with input, hidden, and output layers was generated. The network was limited to one hidden layer and a maximum of five neurons in the hidden layer. A small network with the required accuracy is desirable for the speed of computation.

To validate the networks, the performance plots were generated for all the binary systems. The training and test curves for one representative system is presented in Fig. 1.

The performance plot does not indicate any major problems with the training. The training and test curves are very similar. If the test curves had increased significantly before the training curve increased, then it is possible that some overfitting might have occurred. The best training performance which is represented by the property tr.best\_epoch indicates the iteration at which the validation performance reached a minimum. The training continued for 18 more iteration before the training stopped.

The next step is to evaluate the training state plot. The training record is used to plot the training state plot.

Another plot used to validate the network performance is the error histogram presented in Fig. 2. The error histogram plots a histogram of error values. It computes the error values as the difference between target values and predicted values, helping us to visualize the networks error.

The low values in the error histogram are an indication of a good network performance. The final step in validating the network results is by plotting a regression plot shown in Fig. 3. The solid line in the plot represents the best linear fit regression between outputs and targets.



Fig. 1. Neural network performance plot.



Fig. 2. Neural network error histogram.



Fig. 3. Neural network regression plot.

From Fig. 3, it can be observed that training was perfect. The *R* value of 1 for the training and test data indicates that there is an exact linear relationship between our inputs and targets.

It is important to note that the plots in Figs. 1–3 were obtained after training one of the binary system, and is used to represent the plots obtained when training the entire binary system since similar plots were also obtained for each binary system.

The percentage MAE, and RMSE across each system are presented in Table 1.

The experimental values versus the predicted values for the  $X_i$  and  $Y_i$  for all the 60 binaries denoted (A1–A60) are presented in Figs. 4–15.

Table 1%MAE and %RMSE values across each binary system.

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	no.	Solute	Solute	%MAE X <sub>i</sub>	%MAE Y <sub>i</sub>	%RMSE X <sub>i</sub>	%RMSE Y <sub>i</sub>
2         CO         CH1005         -0.0030         -0.0030         0.0500         0.0041           4         CH20H         CH1005         -0.0220         -0.0321         0.1120         0.1235           5         CH50H         CH1005         0.0007         -0.0038         0.0090         0.0036           6         CH50H         CH1005         0.0000         -0.0035         0.0080         0.0051           7         CH40H         CH1005         -0.0010         -0.0005         0.0080         0.0019           9         H50         CH1007         0.0010         0.0000         0.0001         0.0001           10         CO         Cu8H1         -0.0011         0.0007         0.0070         0.0071           12         H2         Cu8H1         -0.0011         -0.0017         0.0070         0.0071           13         CHOH         Cu8H1         -0.0013         -0.0017         0.0070         0.0071           14         CHOH         Cu8H1         -0.0020         -0.0020         0.0010         0.0018           15         CHOH         Cu8H1         -0.0020         -0.0020         0.0010         0.0015           16         CHOH	1	CO <sub>2</sub>	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	-0.0020	0.0008	0.0210	0.0250
3         H <sub>2</sub> C <sub>H</sub> H <sub>2</sub> O <sub>5</sub> 0.0000         -0.0039         0.0150         0.0451           5         C <sub>H</sub> OH         C <sub>H</sub> H <sub>2</sub> O <sub>5</sub> 0.0002         -0.0005         0.0150         0.0003           6         C <sub>H</sub> OH         C <sub>H</sub> H <sub>2</sub> O <sub>5</sub> 0.0007         -0.0005         0.0040         0.00151           7         C <sub>H</sub> OH         C <sub>H</sub> H <sub>2</sub> O <sub>5</sub> 0.0001         -0.0005         0.0040         0.00151           8         C <sub>H</sub> H <sub>2</sub> OH         C <sub>H</sub> H <sub>2</sub> O <sub>5</sub> 0.0001         -0.0001         0.0000         0.0007           9         H <sub>2</sub> O         C <sub>H</sub> H <sub>2</sub> O <sub>5</sub> 0.0001         -0.0001         0.0007         0.0070         0.0071           10         CO <sub>5</sub> C <sub>H</sub> H <sub>4</sub> 0.0005         -0.0031         0.0040         0.0015           11         CO         C <sub>H</sub> H <sub>4</sub> 0.0012         -0.0031         0.0040         0.0016           116         C <sub>H</sub> SOH         C <sub>H</sub> H <sub>4</sub> -0.0020         0.0010         0.0116           116         C <sub>H</sub> SOH         C <sub>H</sub> H <sub>4</sub> -0.0020         0.0010         0.0116           116         C <sub>H</sub> SOH         C <sub>H</sub> H <sub>4</sub> -0.0010         -0.0023         0.0100         0.0158 <th>2</th> <th>CO</th> <th>C<sub>8</sub>H<sub>18</sub>O<sub>5</sub></th> <th>-0.0030</th> <th>-0.0102</th> <th>0.0560</th> <th>0.0901</th>	2	CO	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	-0.0030	-0.0102	0.0560	0.0901
4         CH <sub>2</sub> OH         C <sub>4</sub> H <sub>2</sub> O <sub>5</sub> -0.0220         -0.0021         0.1120         0.1235           5         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>10</sub> O <sub>5</sub> 0.0007         -0.0038         0.0090         0.0054           7         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>10</sub> O <sub>5</sub> 0.0000         -0.0015         0.0080         0.0015           8         C <sub>4</sub> H <sub>10</sub> OH         C <sub>4</sub> H <sub>10</sub> O <sub>5</sub> 0.0010         0.0007         0.0001         0.0090         0.0015           10         CO         C <sub>4</sub> H <sub>10</sub> O <sub>5</sub> 0.0012         -0.0004         0.0170         0.0071           11         CO         C <sub>4</sub> H <sub>14</sub> 0.0012         -0.0001         0.0070         0.0071           12         H <sub>2</sub> C <sub>4</sub> H <sub>14</sub> 0.0012         -0.0025         0.0210         0.0168           13         CH <sub>2</sub> OH         C <sub>4</sub> H <sub>14</sub> 0.0006         -0.0025         0.0210         0.0169           14         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>14</sub> 0.0005         -0.0026         0.0100         0.0099           15         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>14</sub> -0.0005         -0.0010         0.0009           17         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>14</sub> -0.0007         -0.0010 <t< th=""><th>3</th><th>H<sub>2</sub></th><th>C<sub>8</sub>H<sub>18</sub>O<sub>5</sub></th><th>0.0000</th><th>-0.0039</th><th>0.0150</th><th>0.0451</th></t<>	3	H <sub>2</sub>	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	0.0000	-0.0039	0.0150	0.0451
5         C cH <sub>2</sub> OH         C <sub>4</sub> H <sub>2</sub> OS         0.0020         -0.0005         0.0150         0.0039           6         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> OS         -0.0010         -0.0005         0.0040         0.0019           7         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> OS         0.0019         0.0001         0.0080         0.179           9         H <sub>2</sub> O         C <sub>4</sub> H <sub>4</sub> OS         0.0019         0.0001         0.0080         0.0011           10         CO         C <sub>4</sub> H <sub>4</sub> O         0.0002         -0.0031         0.0007         0.0070         0.0061           11         CO         C <sub>4</sub> H <sub>4</sub> O         0.0012         -0.0031         0.0040         0.0063           12         H <sub>5</sub> C <sub>4</sub> H <sub>6</sub> OH         C <sub>4</sub> H <sub>4</sub> 0.0012         -0.0031         0.0070         0.0068           13         CH <sub>5</sub> OH         C <sub>4</sub> H <sub>4</sub> H         0.0012         -0.0020         0.0070         0.0081           14         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> H         0.0005         -0.0010         0.0010         0.0165           17         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> H <sub>4</sub> -0.0010         -0.0101         0.0000         0.0116           18         H <sub>2</sub> O         C <sub>4</sub> H <sub>4</sub> H <sub>4</sub> -0.0010	4	CH₃OH	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	-0.0260	-0.0321	0.1120	0.1235
6         C <sub>1</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> O <sub>5</sub> 0.0007         -0.0038         0.0090         0.0154           7         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> O <sub>5</sub> 0.0000         -0.0105         0.0080         0.1979           9         H <sub>2</sub> O         C <sub>4</sub> H <sub>4</sub> O <sub>5</sub> 0.0010         0.0099         0.0105           10         CO         C <sub>4</sub> H <sub>4</sub> O <sub>5</sub> 0.0012         -0.0004         0.0107         0.0071           12         H <sub>7</sub> C <sub>4</sub> H <sub>4</sub> O <sub>5</sub> 0.0005         -0.0005         0.0070         0.0063           13         CH <sub>5</sub> OH         C <sub>4</sub> H <sub>4</sub> 0.0013         -0.0017         0.0040         0.0063           14         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> 0.0020         -0.0017         0.0070         0.0081           15         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> 0.0020         -0.0017         0.0070         0.0081           16         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> -0.0020         -0.0014         0.0090         0.0114           17         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>4</sub> -0.0003         0.0002         0.0000         0.0052           18         H <sub>2</sub> O         C <sub>4</sub> H <sub>4</sub> -0.0003         0.0001         0.0253         0.0010 <th>5</th> <th>C<sub>2</sub>H<sub>5</sub>OH</th> <th>C8H18O5</th> <th>0.0020</th> <th>-0.0005</th> <th>0.0150</th> <th>0.0093</th>	5	C <sub>2</sub> H <sub>5</sub> OH	C8H18O5	0.0020	-0.0005	0.0150	0.0093
7         Cid#gOH         Cid#gOG         -0.0010         -0.0005         0.0040         0.0011           8         Cid#nOH         Cid#gOG         0.0019         0.0001         0.0090         0.0105           9         H <sub>2</sub> O         Cid#gOG         0.0019         0.0001         0.0090         0.0011           10         CO2         Cid#gOG         0.0012         -0.0031         0.0040         0.0063           11         Cid         Cid#oH         Cid#gOG         -0.0017         0.0070         0.0063           12         H2         Cig#gOH         Cig#gH         0.0012         -0.0031         0.0040         0.0063           13         CH3OH         Cig#gH         0.0012         -0.0017         0.0070         0.0108           14         Cid#gOH         Cig#gH         -0.0020         -0.0014         0.0090         0.0116           16         Cid#gOH         Cig#gH         -0.0001         -0.0010         0.0100         0.0135           19         CO         CigHa         -0.0010         -0.0010         0.0000         0.0027           21         Co2         CigHa         -0.0010         -0.0010         0.0000         0.0031 <t< th=""><th>6</th><th>C<sub>3</sub>H<sub>7</sub>OH</th><th>C<sub>8</sub>H<sub>18</sub>O<sub>5</sub></th><th>0.0007</th><th>-0.0038</th><th>0.0090</th><th>0.0154</th></t<>	6	C <sub>3</sub> H <sub>7</sub> OH	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	0.0007	-0.0038	0.0090	0.0154
8         Cith. Cith.gob.         0.0000         -0.0105         0.0089         0.0105           10         CO2         Cith.i         0.0022         -0.0004         0.0110         0.0091           11         CO         Cith.ii         -0.0005         -0.0007         0.0070         0.0071           12         H2         Cith.ii         0.0012         -0.0031         0.0040         0.0068           13         CH.OH         Cith.ii         0.0012         -0.0031         0.0040         0.0068           14         Cith.SOH         Cith.SOH         0.0020         -0.0020         0.0070         0.0081           15         Cith.SOH         Cith.SOH         -0.0020         -0.0014         0.0090         0.0160           16         Cith.SOH         Cith.SOH         -0.0039         0.0100         0.0014           17         Cith.SOH         Cith.SOH         -0.0039         0.0100         0.0052           20         H3         Cith.SOH         -0.0001         0.0000         0.0052           21         Cith.SOH         Cith.SOH         0.0001         0.00310         0.0141           21         Cith.SOH         Cith.SOH         0.0001         0.00	7	C4H9OH	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	-0.0010	-0.0005	0.0040	0.0051
9         H <sub>2</sub> O         C <sub>m</sub> H <sub>2</sub> a         0.0019         0.0001         0.0090         0.0105           10         CO         C <sub>m</sub> H <sub>4</sub> 0.0022         -0.0001         0.0070         0.0070           11         CO         C <sub>m</sub> H <sub>4</sub> 0.0012         -0.0031         0.00470         0.0070           13         CH <sub>3</sub> OH         C <sub>m</sub> H <sub>4</sub> 0.0012         -0.0031         0.0040         0.0063           14         C <sub>4</sub> H <sub>2</sub> OH         C <sub>m</sub> H <sub>4</sub> 0.0006         -0.0200         0.0050         0.0011           15         C <sub>4</sub> H <sub>2</sub> OH         C <sub>m</sub> H <sub>4</sub> -0.0020         -0.0030         0.0090         0.0116           16         C <sub>4</sub> H <sub>2</sub> OH         C <sub>m</sub> H <sub>4</sub> -0.0020         -0.0025         0.0100         0.0051           17         C <sub>4</sub> H <sub>2</sub> OH         C <sub>m</sub> H <sub>4</sub> -0.0003         -0.0022         0.0100         0.0158           20         H <sub>2</sub> C <sub>m</sub> H <sub>4</sub> -0.0010         -0.0010         0.0010         0.0052           21         CO <sub>2</sub> C <sub>m</sub> H <sub>4</sub> 0.0002         -0.0011         0.0030         0.0027           22         C <sub>4</sub> H <sub>8</sub> C <sub>1</sub> H <sub>4</sub> -0.0001         -0.0033         0.0040         0.0017<	8	C <sub>5</sub> H <sub>11</sub> OH	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	0.0000	-0.0105	0.0080	0.1979
10         CO         C <sub>10</sub> H <sub>14</sub> 0.0022         −0.0004         0.0070         0.0071           11         CO         C <sub>10</sub> H <sub>14</sub> 0.0005         −0.0005         0.0070         0.0068           13         CH <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0013         −0.0017         0.0070         0.0108           14         C <sub>2</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0013         −0.0017         0.0070         0.0108           15         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0006         −0.0020         0.00050         0.0011           16         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> −0.0020         −0.0026         0.0100         0.0136           17         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> −0.0005         −0.0026         0.0100         0.0053           20         H <sub>2</sub> C <sub>10</sub> H <sub>34</sub> −0.0003         0.0010         0.0054           21         CO         C <sub>10</sub> H <sub>34</sub> −0.0003         0.0002         0.0000         0.0063           22         C <sub>4</sub> H <sub>12</sub> C <sub>10</sub> H <sub>34</sub> −0.0003         0.0004         0.0051           22         C <sub>4</sub> H <sub>14</sub> C <sub>10</sub> H <sub>14</sub> −0.0003         0.0004         0.0051           22	9	H <sub>2</sub> O	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub>	0.0019	0.0001	0.0090	0.0105
11         CO         C <sub>10</sub> H <sub>10</sub> -0.0001         0.0007         0.0070         0.00063           13         CH <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0012         -0.0031         0.0040         0.0063           14         C <sub>2</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0013         -0.0017         0.0070         0.0108           15         C <sub>2</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0006         -0.0020         0.0050         0.00191           16         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>44</sub> -0.0020         -0.0025         0.0110         0.0158           17         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>44</sub> -0.0005         -0.0026         0.0100         0.0059           19         CO         C <sub>10</sub> H <sub>34</sub> -0.0010         -0.0019         0.0310         0.0114           21         CO <sub>2</sub> C <sub>10</sub> H <sub>34</sub> -0.0010         -0.0030         0.0000         0.0052           22         C <sub>4</sub> H <sub>4</sub> C <sub>10</sub> H <sub>34</sub> -0.0001         -0.0030         0.0001         0.0224           23         C <sub>4</sub> H <sub>4</sub> C <sub>10</sub> H <sub>34</sub> -0.0001         0.0233         0.0043         0.0011           24         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0007         0.0010 <t< th=""><th>10</th><th>CO2</th><th>C<sub>10</sub>H<sub>14</sub></th><th>0.0022</th><th>-0.0004</th><th>0.0110</th><th>0.0091</th></t<>	10	CO2	C <sub>10</sub> H <sub>14</sub>	0.0022	-0.0004	0.0110	0.0091
12         Hz         CupHu         0.0005         -0.0003         0.0040         0.0068           13         CH <sub>2</sub> OH         CupHu         0.0013         -0.0017         0.0070         0.0108           15         C <sub>3</sub> H <sub>2</sub> OH         CupHu         0.0013         -0.0017         0.0050         0.0091           16         C <sub>4</sub> H <sub>2</sub> OH         CupHu         -0.0020         -0.0055         0.0100         0.0180           17         C <sub>5</sub> H <sub>1</sub> OH         CupHu         -0.0005         -0.0026         0.0100         0.0059           18         H <sub>2</sub> O         CupHu         -0.0005         -0.0029         0.0100         0.0158           20         H <sub>2</sub> CupHu         -0.0003         0.0002         0.0100         0.0054           21         C0         CupHu         -0.0003         0.0002         0.0000         0.0027           22         C <sub>2</sub> H <sub>6</sub> CupHu         -0.0008         0.0002         0.0030         0.0027           23         C <sub>3</sub> H <sub>2</sub> CupHu         -0.0003         0.00040         0.0051           24         C <sub>4</sub> H <sub>2</sub> CupHu         -0.0003         0.00040         0.0012           25         C <sub>4</sub> H <sub>4</sub> <t< th=""><th>11</th><th>CO</th><th>C<sub>10</sub>H<sub>14</sub></th><th>-0.0001</th><th>0.0007</th><th>0.0070</th><th>0.0071</th></t<>	11	CO	C <sub>10</sub> H <sub>14</sub>	-0.0001	0.0007	0.0070	0.0071
13         CH <sub>3</sub> OH         C <sub>10</sub> H <sub>41</sub> 0.0012         -0.0031         0.0040         0.0063           14         C <sub>3</sub> H <sub>5</sub> OH         C <sub>10</sub> H <sub>41</sub> 0.0006         -0.0020         0.0050         0.0091           15         C <sub>3</sub> H <sub>5</sub> OH         C <sub>10</sub> H <sub>41</sub> -0.0020         -0.0005         0.0210         0.0168           17         C <sub>3</sub> H <sub>1</sub> OH         C <sub>10</sub> H <sub>44</sub> -0.0020         -0.0026         0.0100         0.0090           18         H <sub>2</sub> O         C <sub>10</sub> H <sub>34</sub> -0.0008         -0.0026         0.0100         0.0090           20         H <sub>2</sub> C <sub>10</sub> H <sub>34</sub> -0.0010         -0.0019         0.0110         0.0052           21         CO         C <sub>10</sub> H <sub>34</sub> 0.0002         -0.0001         0.0002         0.0027           22         C <sub>2</sub> H <sub>12</sub> C <sub>10</sub> H <sub>34</sub> -0.0003         0.0002         0.0030         0.0002           23         C <sub>4</sub> H <sub>12</sub> C <sub>10</sub> H <sub>34</sub> -0.0001         -0.2533         0.0404         0.0051           24         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0043         0.0042           28         C <sub>4</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0014         0.0254 </th <th>12</th> <th>H<sub>2</sub></th> <th>C<sub>10</sub>H<sub>14</sub></th> <th>0.0005</th> <th>-0.0005</th> <th>0.0070</th> <th>0.0068</th>	12	H <sub>2</sub>	C <sub>10</sub> H <sub>14</sub>	0.0005	-0.0005	0.0070	0.0068
14         C <sub>H</sub> C <sub>H</sub> C <sub>H</sub> H <sub>14</sub> 0.0013         −0.0017         0.0070         0.0108           15         C <sub>H</sub> H <sub>0</sub> C <sub>H</sub> C <sub>H</sub> H <sub>14</sub> −0.0020         −0.0005         0.0210         0.0160           16         C <sub>H</sub> H <sub>1</sub> OH         C <sub>H</sub> H <sub>14</sub> −0.0050         −0.0025         0.0210         0.0100           17         C <sub>S</sub> H <sub>11</sub> OH         C <sub>H</sub> H <sub>14</sub> −0.0050         −0.0023         0.0100         0.0030           19         CO         C <sub>H</sub> H <sub>34</sub> −0.0010         −0.0039         0.0100         0.0051           20         H <sub>2</sub> C <sub>H</sub> H <sub>34</sub> −0.0010         −0.0010         0.0000         0.0052           21         CO <sub>2</sub> C <sub>H</sub> H <sub>34</sub> −0.0001         −0.0001         0.0000         0.0052           22         C <sub>H</sub> H <sub>3</sub> C <sub>H</sub> H <sub>34</sub> −0.0001         0.0030         0.0027           22         C <sub>H</sub> H <sub>3</sub> C <sub>H</sub> H <sub>34</sub> −0.0001         0.0030         0.0040           23         C <sub>H</sub> H <sub>4</sub> C <sub>H</sub> H <sub>34</sub> −0.00077         0.4030         0.0244           24         C <sub>H</sub> H <sub>34</sub> −0.0030         −0.0016         0.0160         0.0163           24         C <sub>H</sub> H <sub>34</sub>	13	CH₃OH	C <sub>10</sub> H <sub>14</sub>	0.0012	-0.0031	0.0040	0.0063
15         C <sub>3</sub> H <sub>2</sub> OH         C <sub>10</sub> H <sub>14</sub> 0.0006         -0.0020         0.0015         0.0016           16         C <sub>4</sub> H <sub>10</sub> OH         C <sub>10</sub> H <sub>14</sub> -0.0020         -0.0014         0.0090         0.0136           17         C <sub>3</sub> H <sub>10</sub> OH         C <sub>10</sub> H <sub>14</sub> -0.0008         -0.0026         0.0100         0.0039           19         CO         C <sub>10</sub> H <sub>34</sub> -0.0010         -0.0019         0.0310         0.0114           20         H <sub>2</sub> C <sub>10</sub> H <sub>34</sub> -0.0010         -0.0019         0.0310         0.0012           21         CO <sub>2</sub> C <sub>10</sub> H <sub>34</sub> -0.0003         0.0002         0.0030         0.0027           22         C <sub>3</sub> H <sub>8</sub> C <sub>10</sub> H <sub>34</sub> -0.0002         -0.0001         0.0030         0.0043           22         C <sub>3</sub> H <sub>8</sub> C <sub>10</sub> H <sub>34</sub> -0.0003         0.0002         0.0030         0.0043           23         C <sub>3</sub> H <sub>9</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0003         0.0009         0.0160         0.0142           24         C <sub>4</sub> H <sub>10</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0079         0.0430         0.0224           25         C <sub>4</sub> H <sub>9</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0016	14	C <sub>2</sub> H <sub>5</sub> OH	C <sub>10</sub> H <sub>14</sub>	0.0013	-0.0017	0.0070	0.0108
16         C <sub>4</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>14</sub> -0.0020         -0.0015         0.0210         0.0160           17         C <sub>4</sub> H <sub>1</sub> OH         C <sub>4</sub> H <sub>14</sub> -0.0050         -0.0026         0.0100         0.0090           18         H <sub>2</sub> O         C <sub>4</sub> H <sub>14</sub> -0.0008         -0.0026         0.0100         0.0018           20         H <sub>2</sub> C <sub>4</sub> H <sub>34</sub> -0.0010         -0.0019         0.0310         0.0104           21         CO <sub>2</sub> C <sub>4</sub> H <sub>34</sub> 0.0002         -0.0001         0.0000         0.0022           223         C <sub>4</sub> H <sub>8</sub> C <sub>4</sub> H <sub>34</sub> -0.0002         0.0030         0.0027           224         C <sub>4</sub> H <sub>14</sub> C <sub>10</sub> H <sub>34</sub> -0.0002         0.0030         0.0043           255         C <sub>4</sub> H <sub>14</sub> C <sub>10</sub> H <sub>34</sub> -0.0001         -0.2533         1.030         0.4175           276         C <sub>4</sub> H <sub>9</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.001         -0.0080         0.0160         0.0142           28         C <sub>4</sub> H <sub>9</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0077         0.430         0.0294           29         C <sub>4</sub> H <sub>9</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0071         0.0400         0.0013           31         C <sub>4</sub> H	15	C <sub>3</sub> H <sub>7</sub> OH	C <sub>10</sub> H <sub>14</sub>	0.0006	-0.0020	0.0050	0.0091
17       GH <sub>10</sub> OH       C <sub>10</sub> H <sub>14</sub> 0.0009       -0.0014       0.0090       0.0136         18       H <sub>2</sub> O       C <sub>10</sub> H <sub>34</sub> -0.0008       -0.0039       0.0100       0.0158         20       H <sub>2</sub> C <sub>10</sub> H <sub>34</sub> -0.0008       -0.0019       0.0310       0.0141         21       CO <sub>2</sub> C <sub>10</sub> H <sub>34</sub> 0.0002       -0.0001       0.0000       0.0054         223       C <sub>4</sub> H <sub>6</sub> C <sub>10</sub> H <sub>34</sub> 0.0002       -0.0001       0.0000       0.0027         24       C <sub>4</sub> H <sub>4</sub> C <sub>10</sub> H <sub>34</sub> -0.0008       0.0002       0.0030       0.0043         25       C <sub>4</sub> H <sub>14</sub> C <sub>10</sub> H <sub>34</sub> -0.0001       -0.0033       0.0400       0.0051         26       C <sub>11</sub> OH       C <sub>10</sub> H <sub>34</sub> -0.0001       -0.0233       10.030       0.0142         28       C <sub>4</sub> H <sub>7</sub> OH       C <sub>10</sub> H <sub>34</sub> -0.0030       -0.0085       0.0110       0.0193         30       C <sub>4</sub> H <sub>10</sub> OH       C <sub>10</sub> H <sub>34</sub> 0.0032       -0.0172       0.0430       0.0251         33       CO       C <sub>10</sub> H <sub>34</sub> 0.0032       -0.0172       0.0790       0.1900         34       CO <sub>2</sub> C <sub>10</sub> H <sub>30</sub> OH       0.0082	16	C <sub>4</sub> H <sub>9</sub> OH	C <sub>10</sub> H <sub>14</sub>	-0.0020	-0.0005	0.0210	0.0160
H <sub>2</sub> O         Cu <sub>1</sub> H <sub>4</sub> -0.0026         -0.0026         0.0100         0.0108           19         CO         Cu <sub>1</sub> H <sub>34</sub> -0.0008         -0.0019         0.0310         0.0141           21         CD <sub>2</sub> Cu <sub>8</sub> H <sub>34</sub> 0.0002         0.0100         0.0052           22         C <sub>4</sub> H <sub>6</sub> Cu <sub>8</sub> H <sub>34</sub> 0.0002         -0.0001         0.0003         0.0002           23         C <sub>4</sub> H <sub>8</sub> Cu <sub>8</sub> H <sub>34</sub> -0.0008         -0.0001         0.0030         0.0043           24         C <sub>4</sub> H <sub>14</sub> Cu <sub>8</sub> H <sub>34</sub> -0.0002         -0.0003         0.0040         0.0051           26         C <sub>4</sub> H <sub>44</sub> Cu <sub>8</sub> H <sub>34</sub> -0.0001         -0.2533         10.030         0.0142           28         C <sub>4</sub> H <sub>3</sub> OH         Cu <sub>8</sub> H <sub>34</sub> -0.0003         -0.0077         0.0430         0.0294           29         C <sub>4</sub> H <sub>3</sub> OH         Cu <sub>8</sub> H <sub>34</sub> -0.0030         -0.0085         0.0110         0.0193           30         C <sub>4</sub> H <sub>1</sub> OH         Cu <sub>8</sub> H <sub>34</sub> -0.0030         -0.0014         0.0060         0.0056           31         C <sub>4</sub> H <sub>3</sub> OH         Cu <sub>8</sub> H <sub>34</sub> -0.0030         -0.0010         0.0260         0.0071	17	C <sub>5</sub> H <sub>11</sub> OH	C <sub>10</sub> H <sub>14</sub>	0.0009	-0.0014	0.0090	0.0136
19         CO         Cu <sub>B</sub> H <sub>24</sub> −0.0010         −0.0039         0.0100         0.0158           20         H <sub>2</sub> Cu <sub>B</sub> H <sub>24</sub> −0.0010         −0.0010         0.0010         0.0051           21         CO <sub>2</sub> Cu <sub>B</sub> H <sub>24</sub> 0.0002         −0.0001         0.0000         0.0002           23         C <sub>3</sub> H <sub>6</sub> Cu <sub>B</sub> H <sub>24</sub> 0.0002         −0.0001         0.0030         0.0047           24         C <sub>4</sub> H <sub>12</sub> Cu <sub>B</sub> H <sub>24</sub> −0.0002         −0.0003         0.0040         0.0051           25         C <sub>4</sub> H <sub>14</sub> Cu <sub>B</sub> H <sub>24</sub> −0.0002         −0.0003         0.0040         0.0151           26         C <sub>4</sub> H <sub>2</sub> OH         Cu <sub>B</sub> H <sub>24</sub> −0.0000         0.0009         0.0160         0.0142           28         C <sub>4</sub> H <sub>2</sub> OH         Cu <sub>B</sub> H <sub>24</sub> −0.0030         −0.0085         0.0110         0.0193           30         C <sub>4</sub> H <sub>1</sub> OH         Cu <sub>B</sub> H <sub>24</sub> −0.0030         −0.0018         0.0140         0.0056           31         C <sub>4</sub> H <sub>1</sub> OH         Cu <sub>B</sub> H <sub>24</sub> −0.0030         −0.0018         0.0140         0.0051           32         H <sub>2</sub> O         Cu <sub>B</sub> H <sub>24</sub> −0.0030         −0.0010         <	18	H <sub>2</sub> O	C <sub>10</sub> H <sub>14</sub>	-0.0050	-0.0026	0.0100	0.0090
	19	со	C <sub>16</sub> H <sub>34</sub>	-0.0008	-0.0039	0.0100	0.0158
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	20	H <sub>2</sub>	C <sub>16</sub> H <sub>34</sub>	-0.0010	-0.0019	0.0310	0.0141
22         C <sub>3</sub> H <sub>6</sub> C <sub>6</sub> H <sub>34</sub> 0.0002         −0.0001         0.0003         0.0027           23         C <sub>3</sub> H <sub>6</sub> C <sub>6</sub> H <sub>12</sub> C <sub>6</sub> H <sub>14</sub> C <sub>6</sub> H <sub>14</sub> −0.0008         0.0002         0.0030         0.0043           25         C <sub>6</sub> H <sub>14</sub> C <sub>6</sub> H <sub>134</sub> −0.0001         −0.0233         10.030         0.04175           26         CH <sub>3</sub> OH         C <sub>6</sub> H <sub>34</sub> −0.0009         0.0009         0.0160         0.0142           28         C <sub>3</sub> H <sub>7</sub> OH         C <sub>6</sub> H <sub>34</sub> −0.0030         −0.0077         0.0430         0.0294           29         C <sub>4</sub> H <sub>3</sub> OH         C <sub>6</sub> H <sub>34</sub> 0.0034         −0.0070         0.0400         0.0091           30         C <sub>4</sub> H <sub>3</sub> OH         C <sub>6</sub> H <sub>34</sub> 0.0032         −0.0172         0.0790         0.1900           31         C <sub>6</sub> H <sub>30</sub> OH         C <sub>6</sub> H <sub>34</sub> 0.0034         −0.0001         0.0260         0.0071           34         CO <sub>2</sub> C <sub>6</sub> H <sub>33</sub> OH         0.0034         −0.0001         0.0260         0.0079           35         H <sub>2</sub> C <sub>6</sub> H <sub>33</sub> OH         0.0012         0.0004         0.0260         0.0123           36         C <sub>3</sub> H <sub>6</sub> C <sub>6</sub> H <sub>33</sub> OH	21	CO <sub>2</sub>	C <sub>16</sub> H <sub>34</sub>	0.0003	0.0002	0.0100	0.0054
23         C <sub>3</sub> H <sub>8</sub> C <sub>10</sub> H <sub>34</sub> 0.0005         −0.0001         0.0030         0.0027           24         C <sub>4</sub> H <sub>14</sub> C <sub>16</sub> H <sub>34</sub> −0.0002         −0.0003         0.0040         0.0051           25         C <sub>6</sub> H <sub>14</sub> C <sub>16</sub> H <sub>34</sub> −0.0001         −0.2533         10.030         0.4175           27         C <sub>2</sub> H <sub>9</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0009         0.0009         0.0160         0.0142           28         C <sub>4</sub> H <sub>9</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0030         −0.0085         0.0110         0.0193           30         C <sub>5</sub> H <sub>1</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0030         −0.0085         0.0140         0.0091           31         C <sub>6</sub> H <sub>13</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0030         −0.0005         0.0490         0.0071           33         CO         C <sub>16</sub> H <sub>33</sub> OH         0.0032         −0.0005         0.0490         0.0071          34         CO <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH         −0.0055         0.0190         0.0507           36         C <sub>2</sub> H <sub>6</sub> C <sub>16</sub> H <sub>33</sub> OH         −0.0050         0.0423         0.0380         0.2254           37         C <sub>3</sub> H <sub>8</sub> C <sub>16</sub> H <sub>33</sub> OH         −0.0055         0.0190         0.0591     <	22	C <sub>2</sub> H <sub>6</sub>	C <sub>16</sub> H <sub>34</sub>	0.0002	-0.0001	0.0000	0.0052
24         C <sub>9</sub> H <sub>12</sub> C <sub>10</sub> H <sub>34</sub> -0.0008         0.0002         0.0030         0.0043           25         C <sub>4</sub> H <sub>4</sub> C <sub>10</sub> H <sub>34</sub> -0.0001         -0.2533         10.030         0.4175           27         C <sub>4</sub> H <sub>5</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0009         0.0009         0.0160         0.0142           28         C <sub>4</sub> H <sub>5</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0085         0.0110         0.0193           30         C <sub>5</sub> H <sub>1</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0085         0.0110         0.0193           31         C <sub>6</sub> H <sub>1</sub> OH         C <sub>10</sub> H <sub>34</sub> -0.0030         -0.0008         0.0140         0.0091           32         H <sub>2</sub> O         C <sub>10</sub> H <sub>34</sub> 0.0032         -0.0172         0.0790         0.1900           33         CO         C <sub>10</sub> H <sub>33</sub> OH         0.0082         -0.0005         0.04490         0.0071           34         CO <sub>2</sub> C <sub>10</sub> H <sub>30</sub> OH         -0.0010         0.0265         0.0190         0.0507           35         H <sub>2</sub> C <sub>10</sub> H <sub>30</sub> OH         0.0012         0.0004         0.0260         0.0123           36         C <sub>2</sub> H <sub>6</sub> C <sub>10</sub> H <sub>30</sub> OH         0.0050         0.0124	23	C <sub>3</sub> H <sub>8</sub>	C <sub>16</sub> H <sub>34</sub>	0.0005	-0.0001	0.0030	0.0027
25         C <sub>6</sub> H <sub>14</sub> C <sub>16</sub> H <sub>34</sub> −0.0002         −0.0003         0.0040         0.0051           26         CH <sub>2</sub> OH         C <sub>18</sub> H <sub>34</sub> −0.0009         0.0009         0.0160         0.0142           27         C <sub>2</sub> H <sub>5</sub> OH         C <sub>18</sub> H <sub>34</sub> −0.0034         −0.0077         0.0430         0.0294           28         C <sub>3</sub> H <sub>1</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0030         −0.0014         0.0060         0.0091           30         C <sub>3</sub> H <sub>1</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0030         −0.00085         0.0110         0.0091           31         C <sub>6</sub> H <sub>13</sub> OH         C <sub>16</sub> H <sub>34</sub> −0.0030         −0.0005         0.0490         0.0071           33         CO         C <sub>16</sub> H <sub>33</sub> OH         0.0032         −0.0172         0.0790         0.1900           34         CO <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH         0.0034         −0.0005         0.0490         0.0071           35         H <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH         −0.0050         0.0423         0.0380         0.2254           37         C <sub>5</sub> H <sub>6</sub> C <sub>16</sub> H <sub>33</sub> OH         −0.0050         0.0423         0.0380         0.2289           40         C <sub>3</sub> H <sub>6</sub> C <sub>16</sub> H <sub>33</sub> OH         −0.0175         0.0870	24	$C_5H_{12}$	C <sub>16</sub> H <sub>34</sub>	-0.0008	0.0002	0.0030	0.0043
26       CH <sub>3</sub> OH       C <sub>16</sub> H <sub>34</sub> −0.0001       −0.2533       10.030       0.4175         27       C <sub>5</sub> H <sub>5</sub> OH       C <sub>16</sub> H <sub>34</sub> −0.0009       0.0009       0.0160       0.0142         28       C <sub>5</sub> H <sub>5</sub> OH       C <sub>16</sub> H <sub>34</sub> −0.0030       −0.0085       0.0110       0.0193         29       C <sub>4</sub> H <sub>9</sub> OH       C <sub>16</sub> H <sub>34</sub> −0.0030       −0.0014       0.0066       0.0056         31       C <sub>6</sub> H <sub>13</sub> OH       C <sub>16</sub> H <sub>34</sub> 0.00032       −0.0172       0.7990       0.1900         32       H <sub>2</sub> O       C <sub>16</sub> H <sub>34</sub> 0.0032       −0.0005       0.0490       0.0071         34       CO <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH       0.0034       −0.0001       0.0260       0.0079         35       H <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH       −0.0010       0.0055       0.0190       0.0507         36       C <sub>7</sub> H <sub>8</sub> C <sub>16</sub> H <sub>33</sub> OH       0.0012       0.0004       0.0260       0.0123         39       C <sub>4</sub> H <sub>14</sub> C <sub>16</sub> H <sub>33</sub> OH       0.0117       0.0157       0.870       0.2889         40       CH <sub>3</sub> OH       C <sub>16</sub> H <sub>33</sub> OH       0.0007       0.0001       0.0130       0.0078         41       C <sub>3</sub> H <sub>5</sub> OH       C <sub>16</sub> H <sub>33</sub> OH <t< th=""><th>25</th><th><math>C_6H_{14}</math></th><th>C<sub>16</sub>H<sub>34</sub></th><th>-0.0002</th><th>-0.0003</th><th>0.0040</th><th>0.0051</th></t<>	25	$C_6H_{14}$	C <sub>16</sub> H <sub>34</sub>	-0.0002	-0.0003	0.0040	0.0051
27       GH <sub>3</sub> OH       C <sub>16</sub> H <sub>34</sub> -0.0009       0.0009       0.0160       0.0142         28       G <sub>3</sub> H <sub>2</sub> OH       C <sub>16</sub> H <sub>34</sub> -0.0030       -0.0077       0.0430       0.0294         29       C <sub>4</sub> H <sub>3</sub> OH       C <sub>16</sub> H <sub>34</sub> -0.0030       -0.0085       0.0110       0.0193         30       C <sub>4</sub> H <sub>1</sub> OH       C <sub>16</sub> H <sub>34</sub> 0.0032       -0.0172       0.0790       0.1900         31       C <sub>6</sub> H <sub>13</sub> OH       C <sub>16</sub> H <sub>34</sub> 0.0032       -0.0017       0.0790       0.1900         32       H <sub>2</sub> O       C <sub>16</sub> H <sub>33</sub> OH       0.0082       -0.0001       0.0260       0.0079         34       CO <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH       -0.0050       0.0423       0.0380       0.2254         35       H <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH       -0.0050       0.0423       0.0380       0.2254         37       C <sub>3</sub> H <sub>8</sub> C <sub>16</sub> H <sub>33</sub> OH       0.0012       0.0004       0.0260       0.0123         38       C <sub>4</sub> H <sub>14</sub> C <sub>16</sub> H <sub>33</sub> OH       0.0107       0.0157       0.8770       0.2889         40       CH <sub>3</sub> OH       C <sub>16</sub> H <sub>33</sub> OH       0.0005       0.0001       0.0130       0.0276         41       C <sub>3</sub> H <sub>9</sub> OH       C <sub>16</sub> H <sub>33</sub> OH       <	26	CH <sub>3</sub> OH	C <sub>16</sub> H <sub>34</sub>	-0.0001	-0.2533	10.030	0.4175
28         C <sub>3</sub> H <sub>2</sub> OH         C <sub>4</sub> H <sub>3</sub> A         0.0034         -0.0077         0.0430         0.0294           29         C <sub>4</sub> H <sub>9</sub> OH         C <sub>16</sub> H <sub>34</sub> -0.0030         -0.0085         0.0110         0.0193           30         C <sub>9</sub> H <sub>13</sub> OH         C <sub>16</sub> H <sub>34</sub> -0.0030         -0.0014         0.0060         0.0091           31         C <sub>6</sub> H <sub>13</sub> OH         C <sub>16</sub> H <sub>34</sub> 0.0032         -0.0172         0.0790         0.1900           32         H <sub>2</sub> O         C <sub>16</sub> H <sub>33</sub> OH         0.0082         -0.0005         0.0490         0.0071           34         CO <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH         -0.0010         0.0055         0.0190         0.0507           36         C <sub>2</sub> H <sub>6</sub> C <sub>16</sub> H <sub>33</sub> OH         -0.0010         0.00423         0.0380         0.2254           37         C <sub>3</sub> H <sub>8</sub> C <sub>16</sub> H <sub>33</sub> OH         0.0012         0.0044         0.0260         0.0123           39         C <sub>6</sub> H <sub>14</sub> C <sub>16</sub> H <sub>33</sub> OH         0.0107         0.157         0.0870         0.2889           40         CH <sub>3</sub> OH         C <sub>16</sub> H <sub>33</sub> OH         0.0007         -0.0001         0.0150         0.0176           41         C <sub>3</sub> H <sub>7</sub> OH         C <sub>16</sub> H <sub>33</sub> OH         0.0007         -0.012	27	C <sub>2</sub> H <sub>5</sub> OH	C <sub>16</sub> H <sub>34</sub>	-0.0009	0.0009	0.0160	0.0142
2-9C <sub>4</sub> H <sub>9</sub> OHC <sub>16</sub> H <sub>34</sub> 6H <sub>12</sub> OH $-0.0030$ 6H <sub>13</sub> OH $-0.0035$ 0.0014 $0.0110$ 0.0060 $0.0193$ 30C <sub>5</sub> H <sub>13</sub> OHC <sub>16</sub> H <sub>34</sub> 143OH $-0.0030$ 0.0082 0.0005 $-0.0008$ 0.0140 $0.0060$ 0.009131COC <sub>16</sub> H <sub>34</sub> OH 143OH $0.0082$ 0.0082 0.0001 $-0.0005$ 0.0490 $0.0071$ 33COC <sub>16</sub> H <sub>33</sub> OH 143OH $0.0082$ 0.0055 $-0.0005$ 0.0490 $0.0071$ 34CO2 C <sub>2</sub> C <sub>16</sub> H <sub>33</sub> OH 143OH $-0.0010$ 0.0055 $0.0490$ 0.0057 $0.0577$ 36C <sub>2</sub> H <sub>6</sub> C <sub>16</sub> H <sub>33</sub> OH 142 $-0.0010$ 0.0055 $0.0190$ 0.0691 $0.0591$ 38C <sub>3</sub> H <sub>12</sub> C <sub>16</sub> H <sub>33</sub> OH 141 $-0.0004$ 0.0064 $0.0260$ 0.0123 $0.0172$ 0.00870 0.00870 $0.2889$ 40CH <sub>3</sub> OH C <sub>16</sub> H <sub>33</sub> OH 141 $-0.0009$ C <sub>16</sub> H <sub>33</sub> OH 141 $-0.0055$ 0.0011 $0.0130$ 0.00780 $0.0078$ 41C <sub>2</sub> H <sub>5</sub> OH C <sub>16</sub> H <sub>33</sub> OH 141 $-0.0009$ C <sub>16</sub> H <sub>30</sub> OH 143OH $-0.0055$ 0.0001 $0.0140$ 0.0250 $0.0146$ 43C <sub>4</sub> H <sub>10</sub> OH C <sub>16</sub> H <sub>33</sub> OH 143OH $-0.0055$ 0.0006 0.0006 $0.0040$ 0.0125 $0.0173$ 44C <sub>4</sub> H <sub>10</sub> OH C <sub>16</sub> H <sub>33</sub> OH 143OH $-0.0055$ 0.0006 $0.0040$ 0.0125 $0.0173$ 45C <sub>4</sub> H <sub>10</sub> OH C <sub>16</sub> H <sub>33</sub> OH 143OH $-0.0055$ 0.0006 $0.0140$ 0.0125 $0.01663$ 46H <sub>20</sub> C <sub>24</sub> H <sub>58</sub> C 6H <sub>13</sub> OH $-0.0257$ 0.0000 $0.0140$ 0.0000 $0.0000$ 47<	28	C <sub>3</sub> H <sub>7</sub> OH	C <sub>16</sub> H <sub>34</sub>	0.0034	-0.0077	0.0430	0.0294
30 $C_{g}H_{10}H$ $C_{16}H_{34}$ 0.0008-0.00140.00600.000531 $C_{g}H_{10}H$ $C_{16}H_{34}$ -0.0030-0.00080.01400.009132 $H_{2}O$ $C_{16}H_{30}H$ 0.0082-0.01720.07900.190033CO $C_{16}H_{30}H$ 0.0082-0.00050.04900.007134CO2 $C_{16}H_{30}H$ -0.00100.02550.01900.050736 $C_{2}H_{6}$ $C_{16}H_{30}H$ -0.00500.04230.03800.225437 $C_{3}H_{8}$ $C_{16}H_{33}OH$ -0.01070.01570.08700.288940 $C_{4}H_{12}$ $C_{16}H_{33}OH$ 0.00120.00040.02600.012339 $C_{6}H_{14}$ $C_{16}H_{33}OH$ -0.00090.00010.01300.007841 $C_{2}H_{5}OH$ $C_{16}H_{33}OH$ 0.0007-0.00010.00500.014642 $C_{3}H_{9}OH$ $C_{16}H_{33}OH$ 0.0007-0.00010.00500.014643 $C_{4}H_{9}OH$ $C_{16}H_{33}OH$ 0.00050.00660.00400.012545 $C_{6}H_{13}OH$ $C_{00090}$ -0.02870.01400.046346 $H_2O$ $C_{16}H_{33}OH$ -0.02700.06070.12400.000048 $H_2$ $C_{28}H_{58}$ 0.03340.00000.21400.000050 $C_{2}H_{6}$ $C_{28}H_{58}$ 0.00180.00000.01500.000051 $C_{3}H_{5}$ $C_{28}H_{58}$ <t< th=""><th>29</th><th>C<sub>4</sub>H<sub>9</sub>OH</th><th>C<sub>16</sub>H<sub>34</sub></th><th>-0.0030</th><th>-0.0085</th><th>0.0110</th><th>0.0193</th></t<>	29	C <sub>4</sub> H <sub>9</sub> OH	C <sub>16</sub> H <sub>34</sub>	-0.0030	-0.0085	0.0110	0.0193
31 $C_6H_{13}OH$ $C_{16}H_{34}$ $-0.0030$ $-0.0008$ $0.0140$ $0.0091$ 32 $H_2O$ $C_{16}H_{34}$ $0.0032$ $-0.00172$ $0.0790$ $0.1900$ 33 $CO$ $C_{16}H_{33}OH$ $0.0032$ $-0.0005$ $0.0490$ $0.0071$ 34 $CO_2$ $C_{16}H_{33}OH$ $0.0034$ $-0.0001$ $0.0260$ $0.0079$ 35 $H_2$ $C_{16}H_{33}OH$ $-0.0050$ $0.0423$ $0.0380$ $0.2254$ 37 $C_3H_8$ $C_{16}H_{33}OH$ $0.0012$ $0.0004$ $0.0260$ $0.0123$ 38 $C_8H_{12}$ $C_{16}H_{33}OH$ $0.0012$ $0.0004$ $0.0260$ $0.0123$ 40 $CH_3OH$ $C_{16}H_{33}OH$ $0.0017$ $0.0157$ $0.0870$ $0.2289$ 41 $C_2H_5OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0130$ $0.0078$ 41 $C_2H_5OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 43 $C_4H_9OH$ $C_{16}H_{33}OH$ $0.0005$ $0.0100$ $0.0188$ 44 $C_{2H_5OH}$ $C_{16}H_{33}OH$ $-0.0270$ $0.6077$ $0.1210$ $0.1731$ 47 $CO$ $C_{28}H_{58}$ $-0.0120$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.1800$ $0.0000$ 50 $C_2H_6$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0180$ $0.0000$ 51 $C_3H_8$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0170$ </th <th>30</th> <th>C<sub>5</sub>H<sub>11</sub>OH</th> <th>C<sub>16</sub>H<sub>34</sub></th> <th>0.0008</th> <th>-0.0014</th> <th>0.0060</th> <th>0.0056</th>	30	C <sub>5</sub> H <sub>11</sub> OH	C <sub>16</sub> H <sub>34</sub>	0.0008	-0.0014	0.0060	0.0056
32 $H_2 O$ $C_{16}H_{33} H$ 0.0052 $-0.0072$ 0.0790       0.1900         33       CO $C_{16}H_{33} OH$ 0.0082 $-0.0005$ 0.0490       0.0071         34       CO2 $C_{16}H_{33} OH$ 0.0034 $-0.0001$ 0.0260       0.0079         35 $H_2$ $C_{16}H_{33} OH$ $-0.0050$ 0.0423       0.0380       0.2254         37 $C_{2}H_8$ $C_{16}H_{33} OH$ 0.0012       0.0004       0.0260       0.0123         38 $C_{3}H_{12}$ $C_{16}H_{33} OH$ 0.017       0.0157       0.0870       0.2889         40 $CH_3 OH$ $C_{16}H_{33} OH$ 0.0009       0.00011       0.0130       0.0078         41 $C_{2}H_5 OH$ $C_{16}H_{33} OH$ 0.0007 $-0.00011$ 0.0050       0.0146         43 $C_4H_9 OH$ $C_{16}H_{33} OH$ 0.0007 $-0.00011$ 0.0050       0.0146         44 $C_{3}H_7 OH$ $C_{16}H_{33} OH$ $0.0005$ 0.0006       0.0040       0.0125         45 $C_{6}H_{19} OH$ $C_{16}H_{33} OH$ $-0.0270$ 0.6607       0.1210       0.1731	31	С <sub>6</sub> Н <sub>13</sub> ОН	C <sub>16</sub> H <sub>34</sub>	-0.0030	-0.0008	0.0140	0.0091
33         CO $C_{16}H_{33}OH$ 0.0082         -0.0005         0.04490         0.0071           34         CO2 $C_{16}H_{33}OH$ 0.0034         -0.0001         0.02260         0.0079           35         H2 $C_{16}H_{33}OH$ -0.0010         0.0055         0.0190         0.0507           36 $C_{2}H_6$ $C_{16}H_{33}OH$ -0.0050         0.0423         0.0380         0.2254           37 $C_{3}H_8$ $C_{16}H_{33}OH$ 0.0012         0.0004         0.0260         0.0123           38 $C_{3}H_12$ $C_{16}H_{33}OH$ 0.0107         0.0157         0.0870         0.22889           40 $CH_3OH$ $C_{16}H_{33}OH$ 0.0068         -0.0123         0.0740         0.2276           41 $C_{2}H_5OH$ $C_{16}H_{33}OH$ 0.0067         -0.0001         0.0050         0.0146           43 $C_{4}H_9OH$ $C_{16}H_{33}OH$ 0.0007         -0.0027         0.0140         0.0125           44 $C_{3}H_7OH$ $C_{16}H_{33}OH$ 0.0005         0.0006         0.0040         0.0125           45 $C_{6}H_{13}OH$ $C_{16}$	32	H <sub>2</sub> O	$C_{16}H_{34}$	0.0032	-0.01/2	0.0790	0.1900
34         C02         C16 H330H         0.0034 $-0.0001$ 0.0250         0.0079           35         H2         C16H330H $-0.0010$ 0.0055         0.0190         0.0507           36         C2H6         C16H330H $-0.0010$ 0.0025         0.0180         0.2254           37         C3H8         C16H330H         0.0012         0.0042         0.0260         0.0123           39         C6H14         C16H330H         0.0107         0.0157         0.0870         0.2889           40         CH30H         C16H330H $-0.0009$ 0.0001         0.0130         0.0078           41         C2H50H         C16H330H $-0.0099$ 0.0001         0.0050         0.0146           43         C4H30H         C16H330H         0.0007 $-0.0001$ 0.0050         0.0146           44         C4H10H         C16H330H         0.0005         0.0006         0.0040         0.0125           45         C6H30H         C16H330H $-0.0270$ 0.0607         0.1210         0.0731           46         H20         C16H330H $-0.0270$ 0.0600         0.4810         0.0000	33		C <sub>16</sub> H <sub>33</sub> OH	0.0082	-0.0005	0.0490	0.0071
35 $H_2$ $C_{16}H_{33}OH$ $-0.0010$ $0.0055$ $0.0190$ $0.0307$ 36 $C_2H_6$ $C_{16}H_{33}OH$ $-0.0050$ $0.0423$ $0.0380$ $0.2254$ 37 $C_3H_8$ $C_{16}H_{33}OH$ $0.0038$ $-0.0126$ $0.0090$ $0.0691$ 38 $C_5H_{12}$ $C_{16}H_{33}OH$ $0.0012$ $0.0004$ $0.0260$ $0.0123$ 39 $C_6H_{14}$ $C_{16}H_{33}OH$ $0.0107$ $0.0157$ $0.0870$ $0.2889$ 40 $CH_3OH$ $C_{16}H_{33}OH$ $-0.0009$ $0.0001$ $0.0130$ $0.0078$ 41 $C_2H_9OH$ $C_{16}H_{33}OH$ $0.0068$ $-0.0123$ $0.0740$ $0.2276$ 42 $C_3H_7OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 43 $C_4H_9OH$ $C_{16}H_{33}OH$ $0.0005$ $0.0006$ $0.0040$ $0.0125$ 45 $C_6H_{13}OH$ $C_{16}H_{33}OH$ $-0.0270$ $0.6607$ $0.1210$ $0.1731$ 47CO $C_{28}H_{58}$ $-0.0143$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.4810$ $0.0000$ 50 $C_2H_6$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0170$ $0.0000$ 51 $C_3H_8$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0170$ $0.0000$ 52 $C_5H_1H_4$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ 53 $C_6H_{14}$ $C_{28}H_{58}$ $-0.0110$	34		C <sub>16</sub> H <sub>33</sub> OH	0.0034	-0.0001	0.0260	0.0079
30 $C_{2}r_{16}$ $C_{16}r_{13}r_{30}r_{11}$ $-0.0000$ $0.0423$ $0.0380$ $0.2234$ 37 $C_{3}H_{8}$ $C_{16}r_{13}r_{30}H$ $0.0038$ $-0.0126$ $0.0090$ $0.0691$ 38 $C_{5}H_{12}$ $C_{16}H_{30}OH$ $0.0012$ $0.0004$ $0.02260$ $0.0123$ 39 $C_{6}H_{14}$ $C_{16}H_{30}OH$ $0.0009$ $0.0001$ $0.0130$ $0.0078$ 41 $C_{2}H_{5}OH$ $C_{16}H_{33}OH$ $0.0068$ $-0.0123$ $0.0740$ $0.2276$ 42 $C_{3}H_{7}OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 43 $C_{4}H_{9}OH$ $C_{16}H_{33}OH$ $0.0048$ $-0.0055$ $0.0170$ $0.0188$ 44 $C_{5}H_{11}OH$ $C_{16}H_{33}OH$ $0.0048$ $-0.0255$ $0.0140$ $0.0125$ 45 $C_{6}H_{13}OH$ $C_{16}H_{33}OH$ $-0.0270$ $0.0607$ $0.1210$ $0.1731$ 47CO $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.2100$ $0.0000$ 50 $C_2H_6$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 51 $C_3H_8$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0170$ $0.0000$ 52 $C_{2}H_{14}$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ 53 $C_{6}H_{14}$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ 54 $C_{1$	20		С <sub>16</sub> П <sub>33</sub> ОП	-0.0010	0.0055	0.0190	0.0307
57 $C_{3}H_8$ $C_{16}H_{33}OH$ 0.0058 $-0.0125$ 0.0059       0.0059         38 $C_{5}H_{12}$ $C_{16}H_{33}OH$ 0.0012       0.0004       0.0260       0.0123         39 $C_{6}H_{14}$ $C_{16}H_{33}OH$ 0.0107       0.0157       0.0870       0.22889         40 $CH_3OH$ $C_{16}H_{33}OH$ -0.0009       0.0001       0.0130       0.0078         41 $C_{2}H_5OH$ $C_{16}H_{33}OH$ 0.0068       -0.0123       0.0740       0.2276         42 $C_{3}H_7OH$ $C_{16}H_{33}OH$ 0.0007       -0.0055       0.0170       0.0188         44 $C_{5}H_{11}OH$ $C_{16}H_{33}OH$ 0.0005       0.0006       0.0040       0.0125         45 $C_{6}H_{13}OH$ $C_{16}H_{33}OH$ -0.0270       0.6077       0.1210       0.1731         47       CO $C_{28}H_{58}$ 0.0343       0.0000       0.2100       0.0000         48 $H_2$ $C_{28}H_{58}$ 0.0170       0.0000       0.4810       0.0000         50 $C_2H_6$ $C_{28}H_{58}$ 0.0255       0.0000       0.01800       0.0000	27	С <sub>2</sub> п <sub>6</sub>	С <sub>16</sub> П <sub>33</sub> ОП	-0.0050	0.0425	0.0560	0.2234
35 $C_{9}H_{12}$ $C_{16}H_{33}OH$ $0.0012$ $0.0004$ $0.0200$ $0.01123$ 39 $C_{6}H_{14}$ $C_{16}H_{33}OH$ $0.0107$ $0.0157$ $0.0870$ $0.2889$ 40 $CH_{3}OH$ $C_{16}H_{33}OH$ $0.0009$ $0.0001$ $0.0130$ $0.0078$ 41 $C_{2}H_{5}OH$ $C_{16}H_{33}OH$ $0.0068$ $-0.0123$ $0.0740$ $0.2276$ 42 $C_{3}H_{7}OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0055$ $0.0146$ 43 $C_{4}H_{9}OH$ $C_{16}H_{33}OH$ $0.0005$ $0.0006$ $0.0040$ $0.0125$ 45 $C_{6}H_{13}OH$ $C_{16}H_{33}OH$ $-0.0270$ $0.0607$ $0.1210$ $0.1731$ 47C0 $C_{28}H_{58}$ $-0.1100$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0270$ $0.0000$ $0.5600$ $0.0000$ 49CO <sub>2</sub> $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 50 $C_{2}H_{6}$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0180$ $0.0000$ 51 $C_{3}H_{2}$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0170$ $0.0000$ 52 $C_{5}H_{14}$ $C_{28}H_{58}$ $-0.0110$ $0.0000$ $0.0300$ $0.0000$ 54 $CH_{3}OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 55 $C_{2}H_{5}OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 56 $C_{3}H_{7}OH$ $C_{28}$	20			0.0038	-0.0126	0.0090	0.0091
35 $C_{6}H_{14}$ $C_{16}H_{33}OH$ $0.0107$ $0.0107$ $0.0107$ $0.0107$ $0.0107$ $0.0107$ 40 $CH_{3}OH$ $C_{16}H_{33}OH$ $0.0009$ $0.0001$ $0.0130$ $0.0078$ 41 $C_{2}H_{5}OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 42 $C_{3}H_{7}OH$ $C_{16}H_{33}OH$ $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 43 $C_{4}H_{9}OH$ $C_{16}H_{33}OH$ $0.0005$ $0.0006$ $0.0040$ $0.0125$ 45 $C_{6}H_{13}OH$ $C_{16}H_{33}OH$ $-0.0090$ $-0.0287$ $0.0140$ $0.0463$ 46 $H_{2}O$ $C_{16}H_{33}OH$ $-0.0270$ $0.6077$ $0.1210$ $0.1731$ 47CO $C_{28}H_{58}$ $-0.0170$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.2100$ $0.0000$ 49CO <sub>2</sub> $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 50 $C_{2}H_{6}$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 51 $C_{3}H_8$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0150$ $0.0000$ 52 $C_{5}H_{14}$ $C_{28}H_{58}$ $-0.0110$ $0.0000$ $0.0300$ $0.0000$ 54 $CH_3OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 55 $C_{2}H_{7}OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 56 $C_{$	20	C H		0.0012	0.0004	0.0200	0.0123
40CrigonCright30n $-0.0005$ $0.0017$ $0.0130$ $0.0078$ 41C <sub>2</sub> H <sub>5</sub> OHC <sub>16</sub> H <sub>33</sub> OH $0.0005$ $-0.0123$ $0.0740$ $0.2276$ 42C <sub>3</sub> H <sub>7</sub> OHC <sub>16</sub> H <sub>33</sub> OH $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 43C <sub>4</sub> H <sub>9</sub> OHC <sub>16</sub> H <sub>33</sub> OH $0.0048$ $-0.0055$ $0.0170$ $0.0188$ 44C <sub>5</sub> H <sub>11</sub> OHC <sub>16</sub> H <sub>33</sub> OH $0.0005$ $0.0006$ $0.0040$ $0.0125$ 45C <sub>6</sub> H <sub>13</sub> OHC <sub>16</sub> H <sub>33</sub> OH $-0.0090$ $-0.0287$ $0.0140$ $0.0463$ 46H <sub>2</sub> OC <sub>16</sub> H <sub>33</sub> OH $-0.0270$ $0.0607$ $0.1210$ $0.0000$ 48H <sub>2</sub> C <sub>28</sub> H <sub>58</sub> $-0.0170$ $0.0000$ $0.4810$ $0.0000$ 48H <sub>2</sub> C <sub>28</sub> H <sub>58</sub> $0.0343$ $0.0000$ $0.2100$ $0.0000$ 49CO <sub>2</sub> C <sub>28</sub> H <sub>58</sub> $0.0055$ $0.0000$ $0.880$ $0.0000$ 50C <sub>2</sub> H <sub>6</sub> C <sub>28</sub> H <sub>58</sub> $0.0055$ $0.0000$ $0.0180$ $0.0000$ 51C <sub>3</sub> H <sub>8</sub> C <sub>28</sub> H <sub>58</sub> $0.0018$ $0.0000$ $0.0170$ $0.0000$ 52C <sub>5</sub> H <sub>14</sub> C <sub>28</sub> H <sub>58</sub> $-0.0110$ $0.0000$ $0.0300$ $0.0000$ 54CH <sub>3</sub> OHC <sub>28</sub> H <sub>58</sub> $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 55C <sub>2</sub> H <sub>5</sub> OHC <sub>28</sub> H <sub>58</sub> $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 56C <sub>3</sub> H <sub>7</sub> OHC <sub>28</sub> H <sub>58</sub> $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 57C <sub>4</sub> H <sub>9</sub> OH </th <th>3<del>9</del> 40</th> <th>CU-OU</th> <th>C. U. OU</th> <th>0.0107</th> <th>0.0137</th> <th>0.0870</th> <th>0.2885</th>	3 <del>9</del> 40	CU-OU	C. U. OU	0.0107	0.0137	0.0870	0.2885
1 $C_{J}R_{3}OH$ $C_{16}R_{33}OH$ $C_{0000}$ $-0.0012$ $C_{0000}$ $C_{12}T_{000}$ 42 $C_{3}H_{9}OH$ $C_{16}R_{33}OH$ $0.0007$ $-0.0001$ $0.0050$ $0.0146$ 43 $C_{4}H_{9}OH$ $C_{16}H_{33}OH$ $0.0048$ $-0.0055$ $0.0170$ $0.0188$ 44 $C_{5}H_{11}OH$ $C_{16}H_{33}OH$ $0.0005$ $0.0006$ $0.0040$ $0.0125$ 45 $C_{6}H_{13}OH$ $C_{16}H_{33}OH$ $-0.0290$ $-0.0287$ $0.0140$ $0.0463$ 46 $H_{2}O$ $C_{16}H_{33}OH$ $-0.0270$ $0.0607$ $0.1210$ $0.1731$ 47CO $C_{28}H_{58}$ $-0.1100$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.2100$ $0.0000$ 49CO2 $C_{28}H_{58}$ $0.1270$ $0.0000$ $0.5600$ $0.0000$ 50 $C_{2}H_{6}$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 51 $C_{3}H_8$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0170$ $0.0000$ 52 $C_{5}H_{12}$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ 53 $C_{6}H_{14}$ $C_{28}H_{58}$ $-0.0110$ $0.0000$ $0.0300$ $0.0000$ 55 $C_{2}H_{5}OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 56 $C_{3}H_7OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 57 $C_{4}H_9OH$	40	Call-OH	C16H330H	0.0003	_0.0123	0.0130	0.2276
12 $G_{H}OH$ $C_{16}H_{33}OH$ $O.0007$ $O.0071$ $O.0170$ $O.0188$ 43 $C_{4H}OH$ $C_{16}H_{33}OH$ $O.0005$ $O.0006$ $O.0040$ $O.0125$ 44 $C_{5}H_{11}OH$ $C_{16}H_{33}OH$ $O.0005$ $O.0066$ $O.0040$ $O.0125$ 45 $C_{6}H_{13}OH$ $C_{16}H_{33}OH$ $-0.0090$ $-0.0287$ $O.0140$ $O.0463$ 46 $H_2O$ $C_{16}H_{33}OH$ $-0.0270$ $O.0607$ $O.1210$ $O.0000$ 48 $H_2$ $C_{28}H_{58}$ $-0.1100$ $O.0000$ $O.4810$ $O.0000$ 48 $H_2$ $C_{28}H_{58}$ $O.053$ $O.0000$ $O.2100$ $O.0000$ 49 $CO_2$ $C_{28}H_{58}$ $O.0059$ $O.0000$ $O.0880$ $O.0000$ 50 $C_2H_6$ $C_{28}H_{58}$ $O.0055$ $O.0000$ $O.0180$ $O.0000$ 51 $C_{5}H_8$ $C_{28}H_{58}$ $O.0039$ $O.0000$ $O.0170$ $O.0000$ 52 $C_{3}H_{12}$ $C_{28}H_{58}$ $O.0018$ $O.0000$ $O.0170$ $O.0000$ 54 $CH_3OH$ $C_{28}H_{58}$ $-0.0110$ $O.0000$ $O.0300$ $O.0000$ 55 $C_2H_5OH$ $C_{28}H_{58}$ $-0.0030$ $O.0000$ $O.0300$ $O.0000$ 56 $C_3H_7OH$ $C_{28}H_{58}$ $-0.0030$ $O.0000$ $O.0300$ $O.0000$ 57 $C_4H_9OH$ $C_{28}H_{58}$ $O.0022$ $O.0000$ $O.0170$ $O.0000$ 58 $C_5H_{11}OH$ $C_{28}H_{58}$ $O.0022$	42	C <sub>2</sub> H <sub>2</sub> OH	C16H330H	0.0000	-0.00123	0.0050	0.0146
13 $c_{4}r_{3}r_{0}r_{1}$ $c_{16}r_{33}r_{30}r_{1}$ $c_{000}r_{10}$ $c_{0000}r_{10}$ $c_{0000}r_{10}$ $c_{0000}r_{10}$ $c_{0000}r_{10}$ $c_{0000}r_{10}$ $c_{0010}r_{10}$ 44 $c_{5}r_{13}r_{13}OH$ $-0.0090$ $-0.0287$ $0.0140$ $0.0463$ 46 $H_2O$ $c_{16}H_{33}OH$ $-0.0270$ $0.0607$ $0.1210$ $0.1731$ 47CO $c_{28}H_{58}$ $-0.1100$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $c_{28}H_{58}$ $0.0343$ $0.0000$ $0.2100$ $0.0000$ 49CO2 $c_{28}H_{58}$ $0.0059$ $0.0000$ $0.5600$ $0.0000$ 50 $c_{2}H_6$ $c_{28}H_{58}$ $0.0059$ $0.0000$ $0.0180$ $0.0000$ 51 $c_{3}H_8$ $c_{28}H_{58}$ $0.0039$ $0.0000$ $0.0180$ $0.0000$ 52 $c_{3}H_{12}$ $c_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ 53 $c_{6}H_{14}$ $c_{28}H_{58}$ $-0.0040$ $0.0000$ $0.0300$ $0.0000$ 54 $CH_3OH$ $c_{28}H_{58}$ $-0.0110$ $0.0000$ $0.3300$ $0.0000$ 55 $c_{4}H_9OH$ $c_{28}H_{58}$ $-0.0030$ $0.0000$ $0.1870$ $0.0000$ 56 $c_{3}H_7OH$ $c_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 57 $c_{4}H_9OH$ $c_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0170$ $0.0000$ 58 $c_{5}H_{13}OH$ $c_{28}H_{58}$ $0.0002$ $0.0000$ $0.$	43	C.H.OH	CacHapOH	0.0048	-0.0055	0.0170	0.0188
11 $c_{3}h_{10}$ $c_{16}h_{33}$ $c_{0000}$ $c_{0000}$ $c_{0000}$ $c_{0000}$ $c_{0000}$ $c_{0000}$ $c_{00140}$ $c_{00463}$ 45 $c_{6}h_{13}$ OH $-c_{00270}$ $c_{0000}$ $c_{0140}$ $c_{01731}$ $c_{1731}$ 47CO $c_{28}h_{58}$ $-c_{01100}$ $c_{0000}$ $c_{4810}$ $c_{0000}$ 48 $H_2$ $c_{28}h_{58}$ $c_{00343}$ $c_{00000}$ $c_{2100}$ $c_{00000}$ 49CO2 $c_{28}h_{58}$ $c_{01270}$ $c_{00000}$ $c_{5600}$ $c_{00000}$ 50 $c_{2}H_6$ $c_{28}H_{58}$ $c_{00055}$ $c_{00000}$ $c_{00000}$ $c_{00000}$ 51 $c_{3}H_8$ $c_{28}H_{58}$ $c_{00055}$ $c_{00000}$ $c_{000000}$ $c_{00000}$ 52 $c_{5}H_{12}$ $c_{28}H_{58}$ $c_{00039}$ $c_{00000}$ $c_{01100}$ $c_{00000}$ 53 $c_{6}H_{14}$ $c_{28}H_{58}$ $-c_{00110}$ $c_{00000}$ $c_{00000$ $c_{00000}$ 54 $CH_3OH$ $c_{28}H_{58}$ $-c_{00110}$ $c_{00000}$ $c_{03000}$ $c_{00000$ 55 $c_{2}H_5OH$ $c_{28}H_{58}$ $-c_{00300}$ $c_{00000}$ $c_{03000}$ $c_{00000}$ 58 $c_{3}H_1OH$ $c_{28}H_{58}$ $-c_{000300}$ $c_{00000$ $c_{0150}$ $c_{00000$ 59 $c_{6}H_{13}OH$ $c_{28}H_{58}$ $-c_{00150}$ $c_{00000}$ $c_{0340}$ $c_{00000$ 60 $H_2O$ $c_{28}H_{58}$ $-c_{00150}$ $c_{00000}$ $c_{0340}$ $c_{0000$	44	C-HOH	CacHapOH	0.0005	0.0006	0.0040	0.0125
46 $H_2O$ $C_{16}H_{33}OH$ $-0.0270$ $0.0607$ $0.1210$ $0.1731$ 47CO $C_{28}H_{58}$ $-0.1100$ $0.0000$ $0.4810$ $0.0000$ 48 $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.2100$ $0.0000$ 49CO_2 $C_{28}H_{58}$ $0.0270$ $0.0000$ $0.5600$ $0.0000$ 50 $C_2H_6$ $C_{28}H_{58}$ $0.0059$ $0.0000$ $0.0880$ $0.0000$ 51 $C_3H_8$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 52 $C_5H_{12}$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0170$ $0.0000$ 53 $C_6H_{14}$ $C_{28}H_{58}$ $-0.0040$ $0.0000$ $0.0170$ $0.0000$ 54 $CH_3OH$ $C_{28}H_{58}$ $-0.0110$ $0.0000$ $0.0300$ $0.0000$ 55 $C_2H_5OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.1870$ $0.0000$ 56 $C_3H_7OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 57 $C_4H_9OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 58 $C_5H_{11}OH$ $C_{28}H_{58}$ $0.0002$ $0.0000$ $0.0170$ $0.0000$ 59 $C_6H_{13}OH$ $C_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0170$ $0.0000$ 60 $H_2O$ $C_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0340$ $0.0000$	45	C <sub>c</sub> H <sub>12</sub> OH	CicHarOH	-0.0090	-0.0287	0.0140	0.0463
$47$ CO $C_{28}H_{58}$ $-0.1100$ $0.000$ $0.4810$ $0.0000$ $48$ $H_2$ $C_{28}H_{58}$ $0.0343$ $0.0000$ $0.2100$ $0.0000$ $49$ CO2 $C_{28}H_{58}$ $0.1270$ $0.0000$ $0.5600$ $0.0000$ $50$ $C_2H_6$ $C_{28}H_{58}$ $0.0059$ $0.0000$ $0.0880$ $0.0000$ $51$ $C_3H_8$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ $52$ $C_5H_{12}$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0150$ $0.0000$ $53$ $C_6H_{14}$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ $54$ $CH_3OH$ $C_{28}H_{58}$ $-0.0110$ $0.0000$ $0.0300$ $0.0000$ $55$ $C_2H_5OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.1870$ $0.0000$ $56$ $C_3H_7OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.1870$ $0.0000$ $57$ $C_4H_9OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ $58$ $C_5H_{11}OH$ $C_{28}H_{58}$ $0.0002$ $0.0000$ $0.0170$ $0.0000$ $59$ $C_6H_{13}OH$ $C_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0170$ $0.0000$ $60$ $H_2O$ $C_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0340$ $0.0000$	46	H-0	CicHapOH	-0.0270	0.0607	0.1210	0.1731
$48$ $H_2$ $C_{28}H_{58}$ $0.0160$ $0.0000$ $0.2100$ $0.0000$ $49$ $CO_2$ $C_{28}H_{58}$ $0.0250$ $0.0000$ $0.5600$ $0.0000$ $50$ $C_2H_6$ $C_{28}H_{58}$ $0.0059$ $0.0000$ $0.0880$ $0.0000$ $51$ $C_3H_8$ $C_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ $52$ $C_5H_{12}$ $C_{28}H_{58}$ $0.0039$ $0.0000$ $0.0150$ $0.0000$ $53$ $C_{H14}$ $C_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ $54$ $CH_3OH$ $C_{28}H_{58}$ $-0.0040$ $0.0000$ $0.0200$ $0.0000$ $55$ $C_2H_5OH$ $C_{28}H_{58}$ $-0.0110$ $0.0000$ $0.0300$ $0.0000$ $56$ $C_3H_7OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ $57$ $C_4H_9OH$ $C_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ $58$ $C_5H_11OH$ $C_{28}H_{58}$ $0.0022$ $0.0000$ $0.0170$ $0.0000$ $59$ $C_6H_13OH$ $C_{28}H_{58}$ $0.0002$ $0.0000$ $0.0170$ $0.0000$ $60$ $H_2O$ $C_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0340$ $0.0000$	47	CO	CaeHee	-0.1100	0,0000	0.4810	0,0000
49 $\hat{C}_2$ $\hat{C}_{28}H_{58}$ $0.1270$ $0.0000$ $0.5600$ $0.0000$ 50 $\hat{C}_2H_6$ $\hat{C}_{28}H_{58}$ $0.0059$ $0.0000$ $0.0880$ $0.0000$ 51 $\hat{C}_5H_8$ $\hat{C}_{28}H_{58}$ $0.0055$ $0.0000$ $0.0180$ $0.0000$ 52 $\hat{C}_5H_12$ $\hat{C}_{28}H_{58}$ $0.0039$ $0.0000$ $0.0150$ $0.0000$ 53 $\hat{C}_6H_{14}$ $\hat{C}_{28}H_{58}$ $0.0018$ $0.0000$ $0.0170$ $0.0000$ 54 $\hat{C}H_3OH$ $\hat{C}_{28}H_{58}$ $-0.0040$ $0.0000$ $0.0300$ $0.0000$ 55 $\hat{C}_2H_5OH$ $\hat{C}_{28}H_{58}$ $-0.0110$ $0.0000$ $0.3300$ $0.0000$ 56 $\hat{C}_3H_7OH$ $\hat{C}_{28}H_{58}$ $-0.0030$ $0.0000$ $0.3300$ $0.0000$ 57 $\hat{C}_4H_9OH$ $\hat{C}_{28}H_{58}$ $-0.0030$ $0.0000$ $0.0300$ $0.0000$ 58 $\hat{C}_5H_{11}OH$ $\hat{C}_{28}H_{58}$ $0.0002$ $0.0000$ $0.0170$ $0.0000$ 59 $\hat{C}_6H_{13}OH$ $\hat{C}_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0170$ $0.0000$ 60 $H_2O$ $\hat{C}_{28}H_{58}$ $-0.0150$ $0.0000$ $0.0340$ $0.0000$	48	H <sub>2</sub>	C28H58	0.0343	0.0000	0.2100	0.0000
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	49	CO <sub>2</sub>	C <sub>28</sub> H <sub>58</sub>	0.1270	0.0000	0.5600	0.0000
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	50	C <sub>2</sub> H <sub>6</sub>	C <sub>28</sub> H <sub>58</sub>	0.0059	0.0000	0.0880	0.0000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	51	C <sub>3</sub> H <sub>8</sub>	C <sub>28</sub> H <sub>58</sub>	0.0055	0.0000	0.0180	0.0000
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	52	C <sub>5</sub> H <sub>12</sub>	C <sub>28</sub> H <sub>58</sub>	0.0039	0.0000	0.0150	0.0000
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	C <sub>6</sub> H <sub>14</sub>	C <sub>28</sub> H <sub>58</sub>	0.0018	0.0000	0.0170	0.0000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54	CH₃OH	C <sub>28</sub> H <sub>58</sub>	-0.0040	0.0000	0.0200	0.0000
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	55	C <sub>2</sub> H <sub>5</sub> OH	C <sub>28</sub> H <sub>58</sub>	-0.0110	0.0000	0.0300	0.0000
57         C <sub>4</sub> H <sub>9</sub> OH         C <sub>28</sub> H <sub>58</sub> -0.0030         0.0000         0.0300         0.0000           58         C <sub>5</sub> H <sub>11</sub> OH         C <sub>28</sub> H <sub>58</sub> 0.0059         0.0000         0.0150         0.0000           59         C <sub>6</sub> H <sub>13</sub> OH         C <sub>28</sub> H <sub>58</sub> 0.0002         0.0000         0.0170         0.0000           60         H <sub>2</sub> O         C <sub>28</sub> H <sub>58</sub> -0.0150         0.0000         0.0340         0.0000	56	C <sub>3</sub> H <sub>7</sub> OH	C <sub>28</sub> H <sub>58</sub>	0.0042	0.0000	0.1870	0.0000
58         C <sub>5</sub> H <sub>11</sub> OH         C <sub>28</sub> H <sub>58</sub> 0.0059         0.0000         0.0150         0.0000           59         C <sub>6</sub> H <sub>13</sub> OH         C <sub>28</sub> H <sub>58</sub> 0.0002         0.0000         0.0170         0.0000           60         H <sub>2</sub> O         C <sub>28</sub> H <sub>58</sub> -0.0150         0.0000         0.0340         0.0000	57	C <sub>4</sub> H <sub>9</sub> OH	C <sub>28</sub> H <sub>58</sub>	-0.0030	0.0000	0.0300	0.0000
59         C <sub>6</sub> H <sub>13</sub> OH         C <sub>28</sub> H <sub>58</sub> 0.0002         0.0000         0.0170         0.0000           60         H <sub>2</sub> O         C <sub>28</sub> H <sub>58</sub> -0.0150         0.0000         0.0340         0.0000	58	C <sub>5</sub> H <sub>11</sub> OH	C <sub>28</sub> H <sub>58</sub>	0.0059	0.0000	0.0150	0.0000
60 H <sub>2</sub> O C <sub>28</sub> H <sub>58</sub> -0.0150 0.0000 0.0340 0.0000	59	C <sub>6</sub> H <sub>13</sub> OH	C <sub>28</sub> H <sub>58</sub>	0.0002	0.0000	0.0170	0.0000
	60	H <sub>2</sub> O	C <sub>28</sub> H <sub>58</sub>	-0.0150	0.0000	0.0340	0.0000



Fig. 4. Experimental Liquid Mole Fraction versus Predicted Liquid Mole fraction for system A1-A10.



Fig. 5. Experimental Vapor Mole Fraction versus Predicted Vapor Mole fraction for system A1-A10.



Fig. 6. Experimental Liquid Mole Fraction versus Predicted Liquid Mole fraction for system A11-A20.



Fig. 7. Experimental Vapor Mole Fraction versus Predicted Vapor Mole fraction for system A11-A20.



Fig. 8. Experimental Liquid Mole Fraction versus Predicted Liquid Mole fraction for system A21-A30.



Fig. 9. Experimental Vapor Mole Fraction versus Predicted Vapor Mole fraction for system A21-A30.



Fig. 10. Experimental Liquid Mole Fraction versus Predicted Liquid Mole fraction for system A31-A40.





Fig. 12. Experimental Liquid Mole Fraction versus Predicted Liquid Mole fraction for system A41-A50.



Fig. 13. Experimental Vapor Mole Fraction versus Predicted Vapor Mole fraction for system A41-A50.



Fig. 14. Experimental Liquid Mole Fraction versus Predicted Liquid Mole fraction for system A51-A60.



Fig. 15. Experimental Vapor Mole Fraction versus Predicted Vapor Mole fraction for system A51-A60.

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