

## CORRELATIONS

# Structural Group Contribution Method for Predicting the Octane Number of Pure Hydrocarbon Liquids

Tareq A. Albahri<sup>†</sup>

*Chemical Engineering Department, Kuwait University, P.O. Box 5969, Safat 13060, Kuwait*

A theoretical method for predicting the octane number of pure hydrocarbon liquids is presented. The method is based on a structural group contribution approach and requires no experimental procedure or knowledge of the physical or chemical properties only the chemical structure of the molecule. The proposed model is simple and can predict the research and motor octane numbers of more than 200 pure hydrocarbon liquids with an average deviation of 4 and 5.7, respectively. The results of two different sets of structural groups derived from the Joback group contribution approach are tested and compared. The method is notable for the absence of any theoretical procedure which has previously been used to estimate the pure-component octane number. In addition, the method has the potential advantage of synthesis of additional hydrocarbons with knock measurements as a major objective.

### Introduction

The antiknock quality of gasoline is one of its most important properties which set their price. It is normally expressed in terms of octane numbers defined as the volume percentage of isooctane in a blend of *n*-heptane which is equal to the test fuel in knock intensity under standard test conditions. Knocking results from abnormal combustion of fuel leading to pressure surge, loss of power and fuel economy and can result in engine damage.<sup>1</sup>

There are two recognized laboratory engine test methods for evaluating the antiknock quality of motor fuels, namely, the research method (ASTM D908) and the motor method (ASTM D357). Both methods use the same standard test engine but differ in operating conditions. The research octane number (RON), which is representative of the fuel performance during low-speed city driving, is more often reported in the literature than the motor octane number (MON), which is representative of the fuel performance during high-speed highway driving. Correlations developed for estimating octane numbers from other physical and chemical properties are usually based on RON. The calculation of MON from RON has already been established.<sup>2</sup> For pure components both RON and MON are usually reported in databases, most of which are in the gasoline boiling range.<sup>3</sup>

The importance of this work comes from a new generation of molecular models that treat the petroleum fraction not as a bulk of undefined multicomponent mixture but rather as an ensemble of molecular components for the purpose of simulating the kinetics and dynamics of petroleum-refining processes.<sup>4,5</sup> These molecular level models require that the properties of the

ensemble model compounds, whether real or hypothetical, be known in order to calculate the properties of the petroleum fraction feeds and products. This work, which is focused on the prediction of octane number, is a continuation of that effort. We are now in the process of utilizing the same approach to estimate other properties for pure hydrocarbon liquids in the gasoline boiling range.

In addition, we are developing a theoretical procedure that can practically define the molecular composition of petroleum naphtha using a limited set of molecules which when coupled with this method and a proper mixing rule, will provide a good tool for predicting the RON and MON as well as other relevant properties of gasoline. The knowledge accumulated will then be used to estimate the properties of straight-run naphtha and motor gasoline virgin blending stocks with minimal information. The ultimate goal is to incorporate these predictive methods in a molecularly explicit kinetic model with the objective of simulating some key refinery units such as catalytic reforming, alkylation, isomerization, and polymerization for motor gasoline production. Through optimization of operating conditions such as pressure, temperature, catalyst type, and feed and product composition (through blending), such models could potentially improve octane number, reduce pollutants such as benzene and oxygenates, and minimize cost.

Because the quality of gasoline depends on its composition, one could theoretically calculate the octane number from a comprehensive analysis of the individual hydrocarbons in gasoline and their contribution to the overall octane quality. Aside from the fact that a theory describing and quantifying the relationship between composition and octane number has not yet been fully developed, the major obstacles to this approach are in the lack of a method to obtain the compositional data and in the scarcity of octane number ratings for pure hydrocarbons. The former impediment is partially solved

<sup>†</sup> Tel: (+965) 481-7662 (7459). Fax: (+965) 481-1772.  
E-mail: albahri@kuc01.kuniv.edu.kw. Web site:  
<http://www.albahri.info>.

by the introduction of new analytical (gas and liquid chromatography) and theoretical techniques,<sup>4,5</sup> while the latter, which still awaits the introduction of new techniques for estimation, is solved in this work.

Gasoline is a complex mixture of hydrocarbons that boil below 200 °C with hydrocarbon composition ranging from C<sub>4</sub> to C<sub>11</sub>. These hydrocarbons are mainly *n*-paraffins, *i*-paraffins, cyclic compounds, olefins and aromatics.<sup>6</sup> Though gasoline is never analyzed for individual components, around 1500 compounds have been identified so far.<sup>7</sup> The most comprehensive compilation we have seen so far lists the octane numbers of only 200 of these.<sup>3</sup> This makes it necessary to experimentally determine the octane ratings for hundreds of additional compounds, which is not always practical because it requires the use, maintenance, and operation of a costly standard test engine. An estimation technique to predict the octane number of other molecules for which no data are available is therefore essential.

## Background

Octane number is such a sensitive test that there is no satisfactory correlation for it. No method exists for its prediction for pure hydrocarbons as well. Methods available in the literature are usually empirical and predict the octane number of gasoline but from the composition of pure components. Anderson et al.,<sup>8</sup> for example, developed an empirical model for calculating the RON based on chromatographic analysis of gasoline. In their model, the gasoline is divided into 31 hydrocarbon groups or pseudocomponents, all of which are assigned an "effective" octane number that is estimated by regression of experimental data. The octane number of gasoline is calculated by adding the contribution of octane number from each group. Similar procedures that couple chromatographic analysis with regression techniques are proposed by Van Leeuwen et al.,<sup>9</sup> Sasano,<sup>10</sup> and Lugo et al.<sup>11</sup> Although these techniques give reasonably accurate results, they are usually too time-consuming for planning studies and often the compositional data are not available. Ramadhan and Al-Hyali<sup>7</sup> used hydrogen proton nuclear magnetic resonance (<sup>1</sup>H NMR) spectroscopy and regression analysis to predict the octane number of a limited set of pure aromatic compounds. This method requires extensive experimentation and the use of a high-resolution <sup>1</sup>H NMR spectrometer which makes it both expensive and impractical for quick online analysis in addition to limiting it to aromatic compounds only.

Other more simple methods exist in the literature like the Nelson<sup>12</sup> correlation, which requires only the mid-boiling point and either the paraffin content or the Watson characterization factor of gasoline. Baird's<sup>13</sup> correlation requires the API gravity and the final boiling point of the gasoline fraction. Both correlations are graphical and give average deviations of more than 8 octane numbers.

The method of Twu and Coon<sup>14,15</sup> predicts the octane number of a gasoline blend from the olefins, aromatics, and saturates content of each blending stock using binary interaction parameters determined by regression. The method assumes that the octane numbers of olefins, aromatics, and saturates equal the octane number of the parent gasoline. Similar methods based on the total composition of paraffins, naphthenes, and aromatics as correlating parameters were reported by

Rusin et al.,<sup>16</sup> Habib,<sup>17</sup> Cotterman and Plunkee,<sup>18</sup> and Ramadhan and Al-Hyali<sup>19</sup> with varying degrees of success. When this method is used as the basis of the correlation, the results are not very different from those of Nelson and Baird simply because they do not account for the large variation in octane number between isomers. For example, 2-methylheptane has an octane number of 20, whereas 2,2,4-trimethylpentane (also an isooctane) has an octane number of 100. Also, unlike for pure components blending, unless the interaction parameters are based on the properties of the gasoline blending stock like the average boiling point and API gravity for example, they would not have general validity beyond the mixture from which they were determined.

Ramadhan and Al-Hyali<sup>19</sup> calculated the octane number of gasoline using IR and <sup>1</sup>H NMR spectroscopy of the aromatic portion of the gasoline samples and employing regression analysis. The extensive experimental procedure which involves solvent extraction, washing, drying, and distillation, to separate the aromatic portion of the samples, followed by IR and <sup>1</sup>H NMR spectroscopy analysis has a limited potential for adoption and makes the ASTM test more appealing.

So, it is fair to say that, unless the amount of every hydrocarbon in gasoline and their octane number is known, it will be hard to calculate the octane number of the mixture accurately enough. All but one of the above methods is for multicomponent mixtures such as straight-run naphtha, light naphtha, and gasoline. None, however, can predict the octane number for pure components. We believe the method presented here to be the first and only theoretical approach available in the literature to predict the octane number for pure hydrocarbons of all classes, ranging in octane number from -20 to +120 with minimal information and no experimental requirements.

Octane number is one of the most difficult properties to estimate or correlate because of its complex dependency on the molecular structure of the compound. A careful examination of the octane rating of hundreds of hydrocarbons reveals this complex nature. For example, the octane number of *n*-paraffins is a function of the size or number of carbon atoms in the molecule. This simple dependency can easily be translated into a simple correlation function of the boiling point. For more complex compounds such as *i*-paraffins, however, in addition to the total number of carbon atoms, the octane rating depends on the number, type, length, and degree of branching in the molecule, all of which make the correlation with the boiling point alone impossible. In addition to all of the above factors, the octane number for olefins is a function of the number (olefins and diolefins), location (along the chain), orientation (cis/trans), and nature of the bonds (double and triple). The octane number of aromatics is a function of the number and type of benzene rings (condensed and noncondensed), the number of alkyl groups attached to the benzene ring, and their type, length, degree of branching, and location with respect both to the ring and to each other. Cyclic compounds are the most complex because, in addition to all of the above factors, their octane rating is a function of the size and number of cyclic rings, the number, orientation (cis/trans), degree of branching, and location of alkyl groups on the ring and relative to each other. This is further complicated by the coexistence of several of these groups in one

**Table 1. Group Contribution for Estimation of the Octane Number**

HC type	serial no.	group	(RON) <sub>i</sub>	(MON) <sub>i</sub>
paraffins	1	-CH <sub>3</sub>	-2.315	-0.202
	2	>CH <sub>2</sub>	-8.448	-9.082
	3	>CH-	-0.176	-1.821
	4	>C<	11.94	11.90
olefins	5	=CH-	0.392	-2.293
	6	>C=	8.697	2.703
	7	=CH <sub>2</sub>	3.623	-0.254
	8	=C=	-37.37	-42.43
	9	=CH- (cis)	6.269	2.725
	10	=CH- (trans)	6.449	4.743
	11	≡CH	18.36	21.36
	12	≡C-	-7.201	-12.96
cyclic <sup>a</sup>	13	>CH <sub>2</sub>	-4.421	-5.377
	14	>CH-	-2.177	-3.631
	15	>C<	8.916	10.52
	16	=CH-	2.879	-4.765
aromatics <sup>a</sup>	17	>C=	5.409	5.065
	18	=CH-	3.591	9.725
	19	>C=	2.382	-5.650
	20	>C= (o)	-1.768	1.712
	21	>C= (m)	10.24	14.16
	22	>C= (p)	11.51	10.09

<sup>a</sup> Groups 19–22 are all nonfused.

molecule, which makes it difficult to formulate a model that can capture the behavior of all of the different groups of hydrocarbons without taking into account the structure of the molecules. This complex dependency on molecular structure makes correlating the octane number as a function of such physical and chemical properties as the boiling point and Watson characterization factor alone inadequate.<sup>12</sup>

### Structural Group Contribution

The knocking characteristics of pure components should be studied through models that describe the kinetics and dynamics of combustion on a molecular level. However, for our purposes the method presented here suffices. In this work we investigate the structural dependency of the octane number using a structural group contribution approach, which has proven to be a very powerful tool for predicting many physical and chemical properties of pure compounds. The method was successfully used to predict pure-component and mixture properties such as critical temperature, critical pressure, critical volume, boiling point, freezing point, molar volume, viscosity, surface tension, diffusivity, thermal conductivity, heat capacity, heat of formation, heat of combustion, entropy, and Gibbs free energy.<sup>1</sup> Many structural group contribution methods exist in the literature including, but not limited to, the work of Ambrose, Joback, Fedors, Qrrick and Erbar, Grunberg and Nissan, Thin et al., and Benson.<sup>1</sup> The main differences between these are in the choice of the structural groups and the way in which they contribute to the overall property.

We based our choice of groups on the Joback group contribution approach, with some modifications, to account only for the groups that have an influence on the octane number. For example, it was necessary to account for the orientation (cis and trans) of carbon atoms with a double bond in olefins and for the location of the alkyl substitutions on the benzene ring in the ortho, meta, and para positions in aromatics (Table 1). No distinction in the octane rating existed for the cis and trans structural orientations in cyclic compounds. Hence, such a distinction was avoided in the choice of the structural groups. To improve the results, we have

**Table 2. Group Contribution for Estimation of the Octane Number**

HC type	serial no.	group	(RON) <sub>i</sub>	(MON) <sub>i</sub>	
paraffins	1	-CH <sub>3</sub>	0.459	0.491	
	2	-C <sub>2</sub> H <sub>5</sub> (branch)	0.948	0.517	
	3	>CH <sub>2</sub>	0.680	0.722	
	4	α->CH-	-0.139	-0.430	
	5	β->CH-	-0.362	-0.186	
	6	δ->CH-	-0.358	-0.768	
	7	α->C<	-1.357	-1.983	
	8	β->C<	-1.828	-12.88	
	olefins	9	=CH-	-0.078	0.454
		10	=CH- (C# ≥ 5) <sup>a</sup>	-0.660	-4.438
		11	α->C≡	-0.811	-1.542
		12	β->C≡	-0.6441	-1.529
13		=CH <sub>2</sub>	0.119	-1.603	
14		=C=	2.693	4.691	
15		=CH- (cis)	-0.409	-2.414	
16		=CH- (trans)	-0.387	-2.378	
17		≡CH	-1.267	-8.110	
18		≡C-	0.603	-6.501	
cyclic <sup>b</sup>	19	>CH <sub>2</sub>	0.400	-0.105	
	20	>CH-	0.122	1.301	
	21	>CH- (o)	-0.330	1.199	
	22	>C<	-0.800	-3.878	
	23	=CH-	-0.064	0.206	
	24	>C=	-0.356	-9.033	
	25	correction for C <sub>3</sub> ring	-1.217	-2.521	
	26	correction for C <sub>4</sub> ring	1.117	-1.057	
	27	correction for C <sub>7</sub> ring	0.75	2.481	
	28	correction for C <sub>8</sub> ring	-0.468	0.562	
	aromatics <sup>b</sup>	29	=CH-	-0.202	-1.859
		30	>C=	0.193	-1.912
31		>C= (o)	-0.337	-3.151	
32		>C= (m)	-0.959	-3.141	
33		>C= (p)	-0.498	-1.449	

<sup>a</sup> For a carbon atom that is fifth or higher order along the hydrocarbon chain. α-, β-, and δ- refer to the second, third, and fourth positions on the HC chain, respectively. <sup>b</sup> Groups 19–29 are all nonfused.

also accounted for the location of the alkyl branches along the chain for *i*-paraffins and isoolefins, the location of the double bond along the chain in olefins, and the alkyl substitutions and the ring size for cyclic compounds (Table 2).

Rather than identifying both of the double-bonded carbon atoms in olefins with cis and trans orientations as cis and trans structural groups, it was found that the predictions correlate better with the experimental values when these were represented by two structural groups, one identified as cis or trans and the other as normal. These are shown in Table 1 as structural group numbers 5, 9, and 10 and in Table 2 as group numbers 9, 15, and 16.

### Discussion of the Results

In a structural contribution approach, the group contributions are usually incorporated in some form of an equation relating other properties such as boiling point, molecular weight, or just plain constants, to estimate the desired property. Many equations have been proposed ranging from simple relations to complicated polynomials.<sup>1</sup>

We have tested several equations and found the best to predict the octane number in the following form:

$$\text{ON} = a + b\left(\sum_i (\text{ON})_i\right) + c\left(\sum_i (\text{ON})_i\right)^2 + d\left(\sum_i (\text{ON})_i\right)^3 + e\left(\sum_i (\text{ON})_i\right)^4 + f\left(\sum_i (\text{ON})_i\right) \quad (1)$$

where ON is MON or RON,  $\sum_i (\text{ON})_i$  is the sum of the

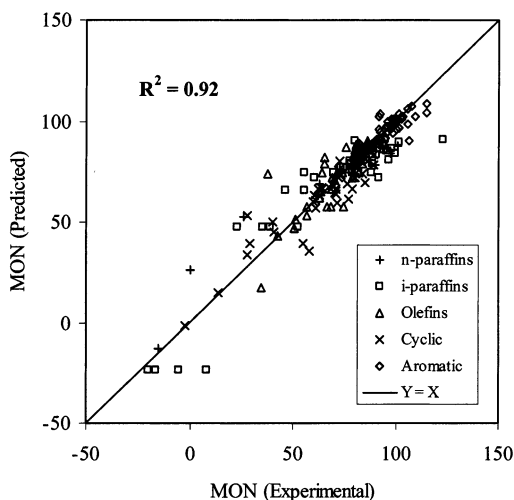
**Table 3. Coefficients for Equation 1**

octane no.	use with Table	a	b	c	d	e	f
RON	1	103.6	0.231	-0.0226	0.001	1.42E-05	1.58
	2	104.8	-5.395	6.532	-5.165	0.6189	-0.0037
MON	1	88.87	0.212	-0.0093	0.00104	9.59E-06	0.339
	2	84.04	1.840	-1.452	-0.357	-0.0179	0

**Table 4. Statistical Analysis for the Octane Number Predictions of Equation 1 in Table 3**

	use Table	octane no. range	correlation coefficient	average deviation <sup>a</sup>	maximum deviation <sup>a</sup>	average % error
RON	1	-20 to +120	0.95	5	29	8
	2		0.975	4	26	6
MON	1		0.92	5.7	45	10
	2		0.84	7.9	48	10

<sup>a</sup> Difference between experimental and calculated octane numbers.

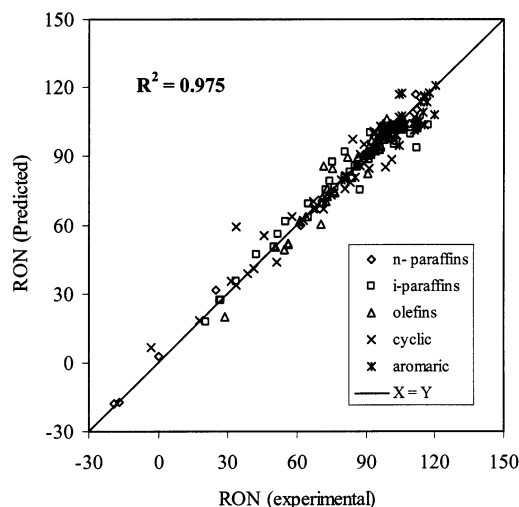
**Figure 1.** Parity plot for the MON of 200 pure hydrocarbon liquids using structural group contributions from Table 1.

group contributions for MON or RON from Tables 1 or 2, respectively, and *a*, *b*, *c*, *d*, *e*, and *f* are correlation constants from Table 3. A sample calculation to illustrate the procedure is presented in the appendix.

Data on the octane number of more than 200 pure components from API-TDB<sup>3</sup> were used to estimate the values of the various group contributions shown in Tables 1 and 2. An optimization algorithm based on the least-squares method was used for that purpose. The algorithm minimizes the sum of the difference between the calculated and experimental octane numbers using the solver function in Microsoft Excel.

Figures 1 and 2 are parity plots for the MON and RON of 200 pure hydrocarbon liquids using structural group contributions from Tables 1 and 2, respectively. It can be seen there that deviation is larger mainly for molecules with MONs below 50. The error analysis is shown in Table 4. Using the minimum number of structural groups to estimate the octane number (Table 1), a correlation coefficient of 0.95 was obtained for RON. This is because of the diverse nature of the octane number which cannot be captured by simple structural models. A better correlation was obtained when more structural groups were used (Table 2). On the contrary, MON correlated better using a fewer number of structural groups from Table 1 than from Table 2. No significant improvement in the model correlation was observed when using separate equations for paraffins, olefins, cyclic compounds, and aromatics, as shown in Table 5.

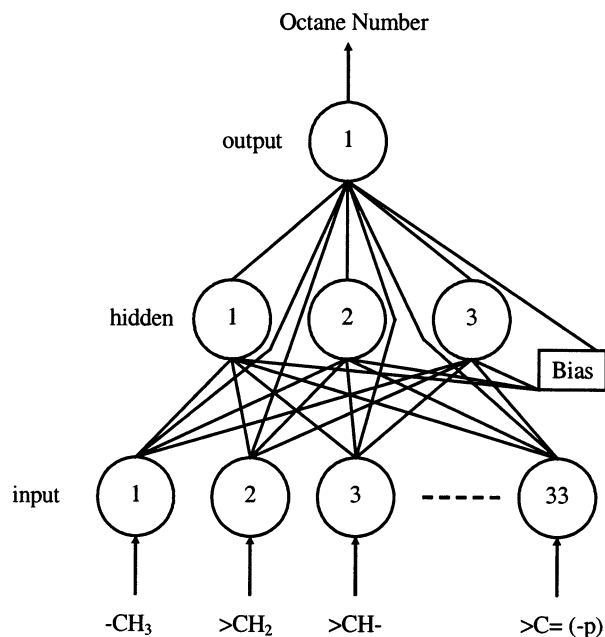
To ascertain the above findings, an artificial neural network was constructed using MATLAB code<sup>20</sup> to

**Figure 2.** Parity plot for the RON of 200 pure hydrocarbon liquids using structural group contributions from Table 2.**Table 5. Statistical Analysis for the RON Predictions of Individual HC Groups**

group	no. of components	correlation coefficient	overall correlation coefficient
<i>n</i> -paraffins	8	0.999	0.978
<i>i</i> -paraffins	43	0.98	
olefins	73	0.97	
cyclic	44	0.99	
aromatics	33	0.97	

predict the octane number of pure hydrocarbon liquids from their structural groups.<sup>4</sup> The network structure is shown in Figure 3 and consists of three layers: input, output, and hidden. The input layer has a number of neurons equal to the number of structural groups shown in either Table 1 or 2. The hidden layer is a single layer with three neurons, and the output layer consists of one neuron. Using the structural groups from Table 1 to predict RON and MON, correlation coefficients of 0.96 and 0.94 were obtained, respectively. This is close to the values from the current group contribution method shown in Table 4 of 0.95 and 0.92, respectively. Using the structural groups from Table 2 to predict RON and MON, correlation coefficients of 0.978 and 0.87 were obtained, respectively. These are close to the values from the current group contribution method of 0.975 and 0.84, respectively.

The comparable deviations and correlation coefficients between the predictions of the two methods<sup>4</sup> negate the possibility of an error instigated by a poor initial guess. They also demonstrate that the present results are



**Figure 3.** Architecture of an artificial neural network for predicting the octane number of pure hydrocarbon liquids from their structural groups.

**Table 6. Testing Set of Components Not Used during Model Development for RON**

compound	ref	RON		deviation <sup>b</sup>
		exptl	pred <sup>a</sup>	
<i>n</i> -octane	6	-19	-17.6	1.4
<i>n</i> -nonane	6	-17	-17.4	0.4
6-methyl-1-heptene	13	63.8	63.4	0.4
2-methyl-2-heptene	13	75.9	74.7	1.2
2,3,4-trimethyl-2-pentene	13	96.9	103	6.1
1,1,2-trimethylcyclopropane	13	113.7	113.2	0.5
1,1,3-trimethylcyclohexane	13	103.5	103.8	0.3
<i>i</i> -butylcyclohexane	13	63.8	63.4	0.4
<i>sec</i> -butylcyclohexane	13	75.9	74.7	1.2

<sup>a</sup> Using eq 1 and Table 2. <sup>b</sup> Average deviation = 1.3.

unlikely to be significantly improved by merely changing eq 1 but would probably require changing the structural group representations themselves.<sup>4</sup> The above results also reveal that MON does not correlate as well as RON. This is probably why most have found it more convenient to predict the RON of gasoline instead of the MON.<sup>8-19</sup>

The fact that fewer groups provided better estimation for MON is further evidence that the structural group contribution approach is not just another correlation technique but in fact a theoretically consistent method for predicting pure-component and multicomponent properties.

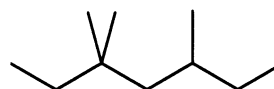
The model is evaluated using a testing set of components not used during development. The components tested and the references from which they were obtained are listed in Tables 6 and 7 for RON and MON, respectively. The model predictions were very accurate with average deviations of 1.3 and 1.5 octane numbers, respectively.

The model appears to be dependent only on the structure of the molecules. Our efforts to include correlating functions using such properties as boiling point, molecular weight, specific gravity, etc., either in the group contributions themselves ( $\sum(\text{ON})_i$ ) or eq 1 did not provide any improvement in the model predictions. This

**Table 7. Testing Set of Components Not Used during Model Development for MON**

compound	ref	MON		
		exptl	pred <sup>a</sup>	deviation <sup>b</sup>
<i>n</i> -octane	6	-15	-13	2.0
6-methyl-1-heptene	13	62.6	61.8	0.8
2-methyl-2-heptene	13	71	69.0	2.0
2,4,4-trimethyl-1-pentene	13	88.6	87.9	0.7
1,1,2-trimethylcyclopropane	13	87.8	87.4	0.4
1,1,3-trimethylcyclohexane	13	82.6	80.9	1.7
2-methylpropene	13	88.1	87.8	0.3
2,5-dimethyl-2,4-hexadiene	13	65.5	81.9	0.2
1-methyl-4-isopropylcyclohexane	13	60.5	63.2	2.7
2-phenyl-1-propene	13	101.3	103.3	2.0
4-methylnonane	13	-20	-23.4	3.4
2,2,6-trimethylheptane	13	78	78.8	0.8

<sup>a</sup> Using eq 1 and Table 1. <sup>b</sup> Average deviation = 1.5.



**Figure 4.** Molecular structure of 3,3,5-trimethylheptane.

is probably because these properties are already incorporated in the structural groups themselves.

## Conclusion and Future Outlook

An estimation technique of the octane rating of pure hydrocarbons, though essential, is nonexistent. The group contribution approach presented here proved to be a powerful tool for predicting the octane number of pure hydrocarbon liquids. This method is useful for the automatic generation and reliable estimation of the octane number of a pure component for which no data exist in the literature, with the objective of estimating the octane number for straight-run and reformer feed naphtha for motor gasoline production. The method is notable for the absence of any theoretical procedure which has previously been used to estimate the octane number of pure hydrocarbon liquids.

We are in the process of developing a theoretical procedure that can practically define the molecular composition of naphtha using a limited set of molecules which, when coupled with this method and a proper mixing rule with interaction parameters, will provide a good tool for predicting the RON and MON of gasoline. We are also developing an algorithm that uses the structural group contributions presented here with the objective of theoretically synthesizing a hydrocarbon liquid with the highest octane number possible for the potential use as an environmentally friendly octane number improver of motor gasoline.

## Acknowledgment

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## Appendix: Sample Calculation

Prediction of the octane number for 3,3,5-trimethylheptane. The molecular structure for 3,3,5-trimethylheptane, shown in Figure 4, consists of the following structural groups obtained from Table 2: five ( $\text{CH}_3$ ), three ( $>\text{CH}_2$ ), one ( $\beta->\text{CH}-$ ) and one ( $\beta->\text{C}<$ ).

Calculation of the overall structural group contributions using Table 2.

$$\begin{aligned} \sum(\text{ON})_i &= 5(\text{CH}_3) + 3(>\text{CH}_2) + 1(\beta->\text{CH}-) + \\ &1(\beta->\text{C}<) = 5(0.459) + 3(0.68) + (-0.362) + \\ &(-1.83) = 2.143 \end{aligned}$$

Substitution into eq 1 with the second row coefficients from Table 3.

$$\begin{aligned} \text{RON} &= 104.8 - 5.395(2.143) + 6.532(2.143)^2 - \\ &5.165(2.143)^3 + 0.6189(2.143)^4 = \\ &85.5 \text{ (experimental 86.4)} \end{aligned}$$

This is only 1 octane number less than the experimental value of 86.4. Note that when using Table 2, the last term  $f$  in eq 1 is insignificant and may be neglected.

### Nomenclature

$i$  = number of structural groups (shown in Tables 1 and 2)  
 MON = motor octane number  
 ON = octane number (either RON or MON)  
 RON = research octane number  
 $\sum(\text{ON})_i$  = summation of the structural group contributions

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