Calculating the Theoretical Octane Number for a Number of Petroleum Derivatives Using Quantum Mechanical Methods AM1 and PM3

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ABSTRACT
This research included calculating a number of physical variables that affect the octane number using semi-empirical methods of quantum mechanics, including AM1, PM3, hardness (η), electron-chemical potential (μ), spherical electrophilic index (W, ΔG, ΔH, ΔS, ΔE and dipole moment). Multiple statistical analyses were used to find the relationship between the calculated variables and the practical value of the octane number and then calculate the octane number theoretically. Through the four-way statistical analysis, we obtained the best correlation coefficient (R2) for the variables (HOMO + η + ΔS + ΔE) calculated by the PM3 method (R2 = 0.998) and the correlation coefficient values for the variables (HOMO + η + W+ μ) calculated by the AM1 method (R2 = 0.980). Through the single and multiple statistical analysis, the most influential variables on the octane number values are (HOMO, LOMO).

1. Introduction

Octane Number

It is a measure of the ignition quality or ignition ability of gasoline and a measure of its anti-knock property. ASTM internal combustion engines are tested under standard conditions. ASTM relies on two different types of octane number values (ON), research octane number (RON), and motor octane number (MON), which are evaluated using (ASTM D2699) and (ASTM D2700) respectively[1,2].

Computational Chemistry

Computational chemistry is one of the branches of physical chemistry, including quantum mechanics and molecular mechanics. Its purpose is to find the most important properties of chemical compounds and compare them with practical values. It is one of the main branches of research used in analysis, diagnosis and support of scientific research[3]. Computational chemistry depends on the use of computers instead of chemicals and the creation of effective mathematical methods to solve theoretical problems through advanced computational methods. John People is considered the first to introduce computers into quantum chemistry in the fifties of the last century by creating new integrated algorithms, highly efficient in calculations, and then marketing computational programs such as the Gaussian program[4]. Computational chemistry is characterized by its easy calculations compared to experiments that are often difficult to perform and involve the risks of chemicals. It is also less expensive because it does not require chemicals and can be performed on any system, even if it is not present, while experiments are limited to relatively stable molecules. However, computational chemistry is not a substitute for experimental methods, but it plays an important role in knowing the properties of chemical compounds[5]. The term computational chemistry is used when the mathematical method has been Develop it sufficiently to be applied using computer programs[6].

Austin Method (AM1)

The AM1 method is one of the distinctive semi-empirical methods due to its widespread use among chemists and its good results, in addition to its availability in most quantum chemistry programs. It represents an extension of the MINDO method or a developed version of it. It was first developed in 1985 by the German scientist Dewar. This method is considered more accurate than the PM3 method in calculating the energy of hydrogen bonds. This method depends on theoretical information as well as interpreting practical results. We can obtain a lot of important information through Modeling organic molecules [7]. such as atomic charges, ionization energy, bond lengths, electron density, values of different angles and formation temperature, but it is not accurate for highly concentrated charges[8].

Parameterized Method (PM3)

The PM3 method uses the same equations used in Austin's AM1 method. The PM3 method is more accurate in calculating hydrogen bond angles compared to the AM1 method. It is considered one of the methods available in all molecular modeling packages that perform semi-empirical calculations. The PM3 method is called the third parameter model (Parameterized Model 3) because it considers that its set of parameters is the third and the first and second are (MNDO, AM1). The theory is still semi- Empirical theory is widely used today not because it competes effectively with more complex theories in terms of accuracy, but because it competes effectively in terms of demand for computational resources. In fact, if one has either a very large molecule, or a large number of small molecules to compare at a fixed level, a semi-empirical theory is considered to have the best solution[9,10].

Theoretical Calculation

In this part of the research, a theoretical study was conducted for a group of compounds using different quantum mechanics methods (AM1, PM3), using these theoretical methods to find the values of the octane number by means of the (Chem. Office) program[11]. and the (Gaussian program Gauss View 06 Gaussian 09) program, where the programs depend on the use of quantum mechanics, which is represented by semi-empirical methods (AM1, PM3), as the programs used in the calculations are one of the modern methods in theoretical calculation chemistry to accomplish theoretical research and support practical research, and the information obtained from using the (Gaussian 09) program is numerous, including: Atomic orbital energy (LUMO), HOMO), dipole moment, temperature of formation, bond lengths, angles between atoms, bond dissociation energy, total energy, charges Atomic, thermodynamic functions, electrostatic potential and energy, transition state structures and their energies .

The program (Gaussian 09) was used as it contains a huge amount of information and this is considered a distinctive thing in calculations using multiple theories in order to conduct a comprehensive search for theoretical methods in the fields of computational chemistry to choose the best of these theories and methods to obtain the best theoretical values for the octane number (ON). In this study, by using Quantum mechanics, which is represented by semi-empirical methods (AM1, PM3), many variables were calculated, which are:

1 - Dipole moment))

2 - Thermodynamic functions (ΔH, ΔG, ΔS, ΔE)

3 - Energy values of atomic orbitals (HOMO, LOMO)

4 - The values of the energy functions that were calculated from the values of (HOMO, LOMO) are {hardness (η), chemical electron potential (μ), and spherical electrophilic index (W)}.

The calculations were carried out using the following methods:

1 - AM1

2 - PM3

Gaussian 09 program

Steps of theoretical calculations for the compounds under study using Gaussian 09

1-Drawing the molecular formula of the compounds using the Chem. Office program).

2-Transferring the compound drawn in the Chem. Office program to the Chem. 3D program).

3-Save the compound in the (Chem. 3D) program in the file format (Input File).

4 - Open the program (6(Gaussian 0. Then open the file saved in (Input File) format.

5 - Select the (Calculate) button, then select (Gaussian Calculation Setup).

6 - From the Job Type button, select (Optimization), then select (Minimum) to obtain the lowest energy, which will be more stable and have the best spatial shape.

7 - After that, from the (Method) button, select the theoretical method and determine the basis set.

8 - After that, select (Submit) to perform the calculations in the (Gaussian 09W) program.

9 - After finishing and completing the results, they will be saved via (Notepad).

10 - The statistical analysis is performed using the SPSS program.

Statistical analysis

Statistical analysis was carried out between the selected and calculated variables (HOMO, LOMO, dipole moment, hardness, electronic potential, spherical electrophilic index, HΔ, GΔ, EΔ, SΔ) using theoretical methods with the practical octane number (ON) values calculated using SPSS program. The values of the correlation coefficient (R^2) were adopted as a reference for this purpose to know the strength and type of relationship between the calculated variables and the practical octane number (ON) values. The statistical analysis was carried out between the variables with each other and with the practical octane number (ON) values using the methods used, where each method was taken separately and with the following steps:

1 - The calculated variables of the studied compounds (HOMO, LOMO, dipole moment, hardness, electronic potential, spherical electrophilic index, ΔH, ΔG, ΔE, ΔS) were entered as non-dependent variables with values The practical octane number that is considered dependent variables.

2 - The variables were analyzed through a series of steps in the SPSS program, using the following steps:

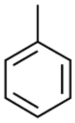
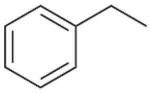
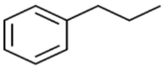
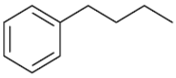
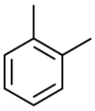
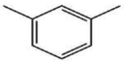
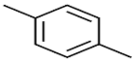
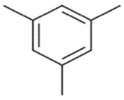
(Linear + regression + analysis)

3 - The values of the correlation coefficient (R^2) are then obtained, since knowing the values of (R^2) determines the variables that have a significant impact on the octane number (ON) in the simple regression analysis.

4 - We then conduct the process of multiple statistical analysis to determine the strength of the relationship between the variables that were used with each other and with the scientific octane number values that were obtained from the literature.

Table 1. Structures of the compounds under study and their names with octane number (ON) values

No.	ON	Nameclature	Structure
1	102	Benzene	

2	122	Toluen	
3	130	Ethyl benzene	
4	110	Propyl benzene	
5	92	Butyl benzene	
6	145	O- Xylene	
7	140	M- Xylene	
8	136	P- Xylene	
9	166	Mesitylene	

Theoretical Calculations

In this research, compounds were studied theoretically and the values of the octane number (ON) were extracted theoretically, as a group of variables were calculated, including the thermodynamic functions (ΔS, ΔE, ΔG, ΔH), the dipole moment, the energy of the orbitals (HOMO, LOMO), and the energy functions (Hardness η, chemical electronic potential μ, spherical electrophilicity index W) The octane number values were calculated for a number of compounds to obtain the best relationship of the variables with each other, and with the octane number values.

Table 2. Calculating the energy values of the studied compounds using the AM1 method

No	**HOMO e.v**	**LOMO e.v**	**η e.v**	**μ e.v**	**W e.v**
1.	- 0.35477	0.02042	0.187595	-0.167175	0.074488872
2.	- 0.34416	0.02002	0.18209	-0.16207	0.072125553
3.	- 0.34352	0.02069	0.182105	-0.161415	0.071537855
4.	- 0.34412	0.01922	0.18167	-0.16245	0.072828559
5.	- 0.34409	0.01920	0.181645	-0.162445	0.072637226
6.	- 0.33288	0.02025	0.176565	-0.156315	0.069193721
7.	- 0.33969	0.02086	0.180275	-0.159415	0.070484377
8.	- 0.33517	0.01959	0.17738	-0.166055	0.077726527
9.	- 0.33784	0.02159	0.179715	-0.158125	0.069564353

Table 3. Calculating the energy values of the studied compounds using the PM3 method

No	**HOMO e.v**	**LOMO e.v**	**η e.v**	**μ e.v**	**W e.v**
1.	- 0.35837	0.01457	0.18647	-0.1719	0.079234219
2.	- 0.34695	0.01434	0.180645	-0.166305	0.07655167
3.	- 0.34618	0.01512	0.18065	-0.16553	0.075837755
4.	- 0.34619	0.01505	0.18062	-0.16557	0.075887013
5.	- 0.34620	0.01502	0.18061	-0.16559	0.075909551
6.	- 0.34173	0.01521	0.17847	-0.16326	0.074673131
7.	- 0.34262	0.01548	0.17905	-0.16357	0.074714171
8.	- 0.33813	0.01431	0.17622	-0.16191	0.074381024
9.	- 0.34053	0.01614	0.178833	-0.1622	0.073756209

Table 4. Calculate thermodynamic functions and dipole moments using the AM1 method

No	**Dipole moment**	**ΔH**	**ΔS**	**ΔG**	**ΔE**
1.	0.0000	0.107727	69.193	0.074851	67.007
2.	0.2471	0.137256	80.308	0.099099	85.537
3.	0.2960	0.167408	85.930	0.126580	104.458
4.	0.3149	0.197475	93.864	0.152877	123.325
5.	0.3185	0.227557	101.866	0.179157	142.201
6.	0.9153	0.152650	87.535	0.111059	95.197
7.	0.2805	0.166796	91.402	0.123367	104.073
8.	0.0003	0.166791	91.383	0.123372	104.071
9.	0.0445	0.196338	102.564	0.147607	122.612

Table 5. Calculate thermodynamic functions and dipole moments using the PM3 method

No	Dipole moment	ΔH	ΔS	ΔG	ΔE
1.	0.0000	0.104250	69.607	0.071177	64.825
2.	0.2502	0.133949	79.949	0.095963	83.462
3.	0.3229	0.163255	84.069	0.123311	101.851
4.	0.3306	0.192538	91.726	0.148956	120.227
5.	0.3355	0.221767	99.534	0.174475	138.568
6.	0.4461	0.164091	85.228	0.123596	102.376
7.	0.2753	0.163659	90.323	0.120744	102.105
8.	0.0002	0.163653	90.279	0.120759	102.102
9.	0.0347	0.193377	100.708	0.145527	120.753

Table 6. Descriptive statistics for study variables calculated using the AM1 method

AM1	ON	Dipole moment	ΔH	ΔS	ΔG	ΔE	HOMO	LOMO	η	μ	W
Mean	127	0.2686	0.1689	89.3383	0.1264	105.3868	-0.3418	0.0202	0.1810	-0.1617	0.0723
Std. Error of Mean	8	0.0927	0.0118	3.4622	0.0103	7.4058	0.0021	0.0003	0.0011	0.0012	0.0009
Median	130	0.2805	0.1668	91.3830	0.1234	104.0730	-0.3435	0.0203	0.1816	-0.1621	0.0721
Std.div.	23	0.2781	0.0354	10.3865	0.0308	22.2175	0.0064	0.0008	0.0032	0.0035	0.0026
Variance	534	0.0770	0.0010	107.879	0.0010	493.6180	0.0000	0.0000	0.0000	0.0000	0.0000
Range	74	0.9153	0.1198	33.3710	0.1043	75.1940	0.0219	0.0024	0.0110	0.0109	0.0085
Minimum	92	0.0000	0.1077	69.1930	0.0749	67.0070	-0.3548	0.0192	0.1766	-0.1672	0.0692
Maximum	166	0.9153	0.2276	102.564	0.1792	142.2010	-0.3329	0.0216	0.1876	-0.1563	0.0777

Table 7. Descriptive statistics for study variables calculated using the PM3 method

PM3	ON	Dipole moment	ΔH	ΔS	ΔG	ΔE	HOMO	LOMO	η	μ	W
Mean	127	0.2217	0.1667	87.9359	0.1249	104.0299	-0.3452	0.0150	0.1802	-0.1651	0.0757
Std. Error of Mean	8	0.0556	0.0114	3.2172	0.0100	7.1781	0.0019	0.0002	0.0009	0.0010	0.0005

Median	130	0.2753	0.1637	90.2790	0.1233	102.1050	-0.3462	0.0151	0.1806	-0.1655	0.0758
Std.div.	23	0.1667	0.0343	9.6516	0.0300	21.5344	0.0058	0.0006	0.0028	0.0030	0.0016
Variance	534	0.0280	0.0010	93.1530	0.0010	463.7320	0.0000	0.0000	0.0000	0.0000	0.0000
Range	74	0.4461	0.1175	31.1010	0.1033	73.7430	0.0202	0.0018	0.0103	0.0100	0.0055
Minimum	92	0.0000	0.1043	69.6070	0.0712	64.8250	-0.3584	0.0143	0.1762	-0.1719	0.0738
Maximum	166	0.4461	0.2218	100.7080	0.1745	138.5680	-0.3381	0.0161	0.1865	-0.1619	0.0792

Table 8. Pearson correlation coefficient values between variables calculated by AM1 method

DFT		**ON**	**Dipole moment**	**ΔH**	**ΔS**	**ΔG**	**ΔE**	**HOMO**	**LOMO**	**η**	**μ**	**W**
ON	**R**	1	0.098	-0.019	0.287	-0.068	-0.019	.717*	.729*	-0.631	0.629	-0.44
	p		0.803	0.961	0.453	0.862	0.961	0.03	0.026	0.068	0.07	0.236
Dipole moment	**R**	0.098	1	0.066	0.073	0.064	0.066	0.447	-0.139	-0.467	.682*	-0.586
	p	0.803		0.866	0.851	0.87	0.866	0.228	0.722	0.205	0.043	0.098
ΔH	**R**	-0.019	0.066	1	.942**	.999**	1.000**	0.338	-0.258	-0.372	0.3	-0.167
	p	0.961	0.866		0	0	0	0.374	0.503	0.324	0.433	0.668
ΔS	**R**	0.287	0.073	.942**	1	.922**	.942**	0.568	-0.046	-0.577	0.46	-0.258
	p	0.453	0.851	0		0	0	0.111	0.906	0.104	0.213	0.503
ΔG	**R**	-0.068	0.064	.999**	.922**	1	.999**	0.297	-0.289	-0.335	0.271	-0.15
	p	0.862	0.87	0	0		0	0.437	0.45	0.378	0.481	0.699
ΔE	**R**	-0.019	0.066	1.000**	.942**	.999**	1	0.338	-0.258	-0.372	0.3	-0.167
	p	0.961	0.866	0	0	0		0.374	0.503	0.324	0.433	0.668
HOMO	**R**	.717*	0.447	0.338	0.568	0.297	0.338	1	0.113	-.992**	0.63	-0.258
	p	0.03	0.228	0.374	0.111	0.437	0.374		0.773	0	0.069	0.502
LOMO	**R**	.729*	-0.139	-0.258	-0.046	-0.289	-0.258	0.113	1	0.011	0.447	-0.549
	p	0.026	0.722	0.503	0.906	0.45	0.503	0.773		0.978	0.227	0.126
η	**R**	-0.631	-0.467	-0.372	-0.577	-0.335	-0.372	-.992**	0.011	1	-0.578	0.192
	p	0.068	0.205	0.324	0.104	0.378	0.324	0	0.978		0.103	0.621
μ	**R**	0.629	.682*	0.3	0.46	0.271	0.3	0.63	0.447	-0.578	1	-.911**
	p	0.07	0.043	0.433	0.213	0.481	0.433	0.069	0.227	0.103		0.001
W	**R**	-0.44	-0.586	-0.167	-0.258	-0.15	-0.167	-0.258	-0.549	0.192	-.911**	1

	p	0.236	0.098	0.668	0.503	0.699	0.668	0.502	0.126	0.621	0.001	

R: Pearson correlation, P: p value

*Correlation is significant at the 0.05 level.

**Correlation is significant at the 0.01 level

Table 9. Pearson correlation coefficient values between variables calculated by PM3 method

DFT		**ON**	**Dipole moment**	**ΔH**	**ΔS**	**ΔG**	**ΔE**	**HOMO**	**LOMO**	**η**	**μ**	**W**
ON	**R**	1	-0.152	0.043	0.29	0.005	0.043	.679*	0.571	-0.611	.709*	-.743*
	p		0.696	0.912	0.449	0.99	0.912	0.044	0.108	0.081	0.033	0.022
Dipole moment	**R**	-0.152	1	0.362	0.139	0.393	0.362	0.133	0.141	-0.149	0.142	-0.153
	p	0.696		0.338	0.721	0.296	0.338	0.734	0.717	0.703	0.716	0.695
ΔH	**R**	0.043	0.362	1	.940**	.999**	1.000**	0.557	0.509	-0.511	0.586	-0.62
	p	0.912	0.338		0	0	0	0.119	0.161	0.16	0.097	0.075
ΔS	**R**	0.29	0.139	.940**	1	.920**	.940**	.706*	0.596	-0.645	.738*	-.774*
	p	0.449	0.721	0		0	0	0.033	0.091	0.061	0.023	0.014
ΔG	**R**	0.005	0.393	.999**	.920**	1	.999**	0.529	0.491	-0.485	0.556	-0.59
	p	0.99	0.296	0	0		0	0.143	0.18	0.186	0.12	0.094
ΔE	**R**	0.043	0.362	1.000**	.940**	.999**	1	0.557	0.509	-0.511	0.586	-0.62
	p	0.912	0.338	0	0	0		0.119	0.161	0.16	0.097	0.075
HOMO	**R**	.679*	0.133	0.557	.706*	0.529	0.557	1	0.336	-.990**	.996**	-.974**
	p	0.044	0.734	0.119	0.033	0.143	0.119		0.376	0	0	0
LOMO	**R**	0.571	0.141	0.509	0.596	0.491	0.509	0.336	1	-0.204	0.42	-0.54
	p	0.108	0.717	0.161	0.091	0.18	0.161	0.376		0.599	0.261	0.133
η	**R**	-0.611	-0.149	-0.511	-0.645	-0.485	-0.511	-.990**	-0.204	1	-.973**	.933**
	p	0.081	0.703	0.16	0.061	0.186	0.16	0	0.599		0	0
μ	**R**	.709*	0.142	0.586	.738*	0.556	0.586	.996**	0.42	-.973**	1	-.991**
	p	0.033	0.716	0.097	0.023	0.12	0.097	0	0.261	0		0
W	**R**	-.743*	-0.153	-0.62	-.774*	-0.59	-0.62	-.974**	-0.54	.933**	-.991**	1
	p	0.022	0.695	0.075	0.014	0.094	0.075	0	0.133	0	0	

R: Pearson correlation, P: p value

*Correlation is significant at the 0.05 level.

**Correlation is significant at the 0.01 level

Table 10. Values of the correlation coefficient (R^2) between the octane number and the variables calculated in the quadratic statistic using the (AM1) method.

Model	**Variables**	**R^2**

No.		
1	HOMO+LOMO+η+W	0.951
2	HOMO+η +W+ μ	0.980
3	HOMO + η+ ΔS + ΔE	0.953
4	HOMO+η + ΔE +LOMO	0.946
5	ΔE + HOMO + ΔG+ μ	0.930
6	ΔE+ LOMO+μ +W	0.963
7	ΔE + W+HOMO+ΔG	0.867
8	LOMO + ΔS+G Δ +W	0.890
9	W+ LOMO+ ΔS+ΔH	0.890
10	W+ ΔS + ΔH +HOMO	0.867

Table 11. Values of the correlation coefficient (R^2) between the octane number and the variables calculated in the quadratic statistic using the (PM3) method.

Model No.	Variables	R^2
1	HOMO+LOMO+η+W	0.667
2	HOMO+η +W+ μ	0.669
3	HOMO + η+ ΔS + ΔE	0.998
4	HOMO+η + ΔE +LOMO	0.987
5	ΔE + HOMO + ΔG+ μ	0.981
6	ΔE+ LOMO+μ +W	0.962
7	ΔE + W+HOMO+ΔG	0.963
8	LOMO + ΔS+G Δ +W	0.963
9	W+ LOMO+ ΔS+ΔH	0.963
10	W+ ΔS + ΔH +HOMO	0.963

Calculating the theoretical octane number values

The four-quadrant statistical regression coefficient values were used to estimate the octane number values through the appropriate statistical model for each of the four methods:

$$Theoritical\ Octan\ No. = Constant + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 + error$$

Calculating theoretical octane number values using the AM1 method

From Table (10), the second model was identified as the best model for calculating the values of the theoretical octane number, because the R^2 values were the highest value compared to the other models, by an amount of 0.980. The table shows the estimation of the four-statistics model parameters using the AM1 method for calculating the octane number. Table (12) shows the coefficients determined by the model, which include variables such as HOMO, LOMO, W, μ. The table also shows the standardized values and (Standardized Coefficients) which show the effect of each variable in a standard way, where Beta shows the effect of each variable in relation to the adopted variable in a standard way. Statistical test and p value. It also shows how influential each variable is in relation to the model statistically.

Table 12. Estimating parameters for the quadrilateral statistical model used to calculate the octane number using the AM1 method

Methods	Model	Coefficients	Unstandardized	Standardized	t	P

			Coefficients		**Coefficients**		**value**
			B	**Std. Error**	**Beta**		
AM1	**Model 2**	(Constant)	362.202	123.521	-	2.932	.043
		HOMO	- 11869.710	6092.002	-3.306	-1.948	.123
		LOMO	37324.747	7329.800	1.281	5.092	.007
		W	70268.927	29479.015	8.026	2.384	.076
		µ	62615.144	26697.926	9.453	2.345	.079

Table (13) reflects the performance of the quadrilateral statistical model using the AM1 method to calculate the octane number. The results show that this second model has a very strong relationship with the correlation coefficient (R = 0.990), with the square value of the correlation coefficient (R^2 = 0.980) indicating that 98% of the variation in octane number can be explained by the independent variables used. The Adjusted R^2 value (0.959) reflects the accuracy of the model based on the number of variables and sample size, while the standard error of the estimate (Std. Error of the Estimate = 4.670) shows the amount of expected deviation between actual values and forecasts. Overall, the table shows that the model has excellent ability to predict octane number based on the independent variables, with the standard error of the estimate needing to be taken into account in evaluating its accuracy.

Table 13. Characteristics of the quadrilateral statistical model used to calculate the octane number using the AM1 method

Model Summary					
Methods	Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
AM1	Model 2	.990	.980	.959	4.670

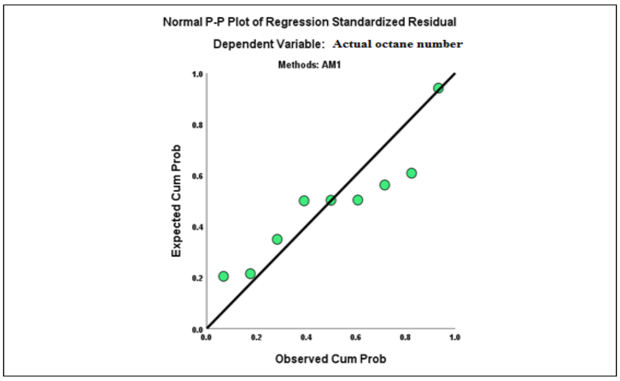


Figure1. Normal P-P plot of regression standardized residual

Therefore, the statistical model equation is formed by substituting the estimates of the second component into equation (1) as follows:

$$\text{Theoritical Octan No.} = 362.202 - (11869.710 * \text{HOMO}) + (37324.747 * \text{LOMO}) + (70268.927 * \text{W}) + (62615.144 * \mu) + \text{error}$$

The results of Table (14) show the theoretical values of octane numbers calculated using the AM1 method, where the accuracy of the predictions reflects excellent results. The differences (Δ) between the actual and theoretical values indicate a strong agreement, especially in compound 3 which shows a small difference (2), which reflects high accuracy. Even in cases with larger differences, such as Compound 2, the results remain encouraging and open the way for additional improvements. Values associated with molecular properties, such as μ, W, LOMO, η, and HOMO, enhance our understanding of the factors influencing octane number estimates. Overall, the results are excellent and demonstrate the effectiveness of the AM1 method in estimating octane numbers for a variety of compounds.

Table (14). Theoretical octane number values for the AM1 method

Compound	*HOMO*	*LOMO*	*W*	µ	Theoretical octane number	True Octane Number	Δ
1	-0.35477	0.02042	0.07449	-0.16718	102	102	0
2	-0.34416	0.02002	0.07213	-0.16207	115	122	7
3	-0.34352	0.02069	0.07154	-0.16142	132	130	2
4	-0.34412	0.01922	0.07283	-0.16245	110	110	0
5	-0.34409	0.01920	0.07264	-0.16245	96	92	4
6	-0.33288	0.02025	0.06919	-0.15632	144	145	1
7	-0.33969	0.02086	0.07048	-0.15942	144	140	4
8	-0.33517	0.01959	0.07773	-0.16606	136	136	0
9	-0.33784	0.02159	0.06956	-0.15813	165	166	1

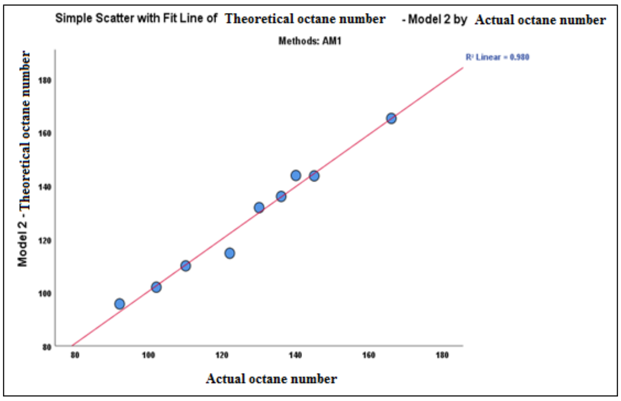


Figure 2. Simple Scatter plot with fit line for model 2

Calculating theoretical octane number values using the PM3 method

From Table (11), the third model was identified as the best model for calculating the theoretical octane number values because the R^2 values were the highest value compared to the other models by 0.998. Table (15) shows the estimation of the parameters of the quadrilateral statistical model using the MP3 method to calculate the octane number. The table shows the coefficients for the variables determined by the model, where the variables include: HOMO, η, ΔS, and ΔE. The table also shows the Standardized Coefficients, which show the effect of each variable in a standard way, where Beta shows the effect of each variable in relation to the adopted variable. Statistical test and p value. It also shows how influential each variable is in relation to the model statistically.

Table 15. Quaternary statistics of octane number using the PM3 method

Methods	**Model**	**Coefficients**	**Unstandardized Coefficients**	**Standardized**	**Statistical test**	**P value**

					Coefficients		
			B	**Std. Error**	**Beta**		
PM3	**Model 3**	(Constant)	1305.677	65.328	-	19.987	<0.001
		HOMO	25030.987	1049.446	6.295	23.852	<0.001
		η	42249.108	1955.718	5.095	21.603	<0.001
		Δ S	-1.217	0.289	-0.508	-4.207	0.014
		ΔE	-0.412	0.099	-0.385	-4.146	0.014

Table (16) reflects the performance of the quadrilateral statistical model using the MP3 method to calculate the octane number. The results show that this third model has a very strong relationship with the correlation coefficient ($R = 0.999$), with the squared value of the correlation coefficient ($R^2 = 0.998$) indicating that 99.8% of the variation in octane number can be explained by the independent variables used. Adjusted R^2 values (0.959) reflect the accuracy of the model based on the number of variables and sample size, while the standard error of the estimate (Std. Error of the Estimate = 1.628) shows the amount of expected deviation between actual values and forecasts. Overall, the table shows that the model has excellent ability to predict octane number based on the independent variables, with the standard error of the estimate needing to be taken into account in evaluating its accuracy.

Table 16. Characteristics of the quadrilateral statistical model used to calculate the octane number using the MP3 method

Model Summary					
Methods	Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
PM3	Model 3	0.999	0.998	0.995	1.628

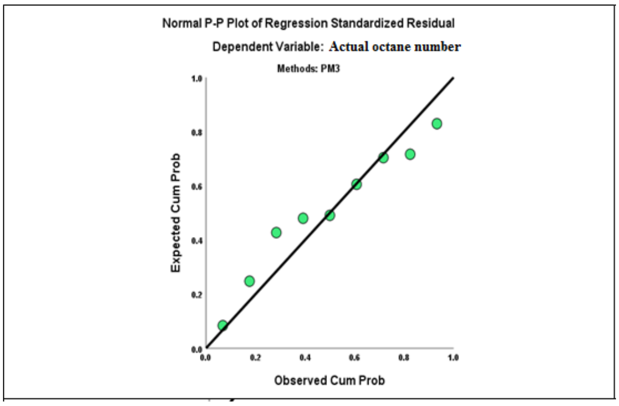


Figure 3. Normal P-P plot of regression standardized residual

Therefore, the statistical model equation is formed by substituting the estimates of the third component into equation (1) as follows:

$$\text{Theoritical Octan No.} = 1305.677 - (25030.987 * \text{HOMO}) + (42249 * \eta) - (1.217 * \Delta S) - (0.412 * \Delta E) + \text{error}$$

Table 17. Theoretical octane number values for the MP3 method

Compound	*HOMO*	η	ΔS	ΔE	Theoretical octane number	True Octane Number	Δ
1	-0.35837	0.186470	69.607	64.825	102	102	0
2	-0.34695	0.180645	79.949	83.462	122	122	0
3	-0.34618	0.180650	84.069	101.851	128	130	2
4	-0.34619	0.180620	91.726	120.227	110	110	0
5	-0.34620	0.180610	99.534	138.568	92	92	0
6	-0.34173	0.178470	85.228	102.376	146	145	1
7	-0.34262	0.179050	90.323	102.105	142	140	2
8	-0.33813	0.176220	90.279	102.102	135	136	1
9	-0.34053	0.178833	100.708	120.753	165	166	1

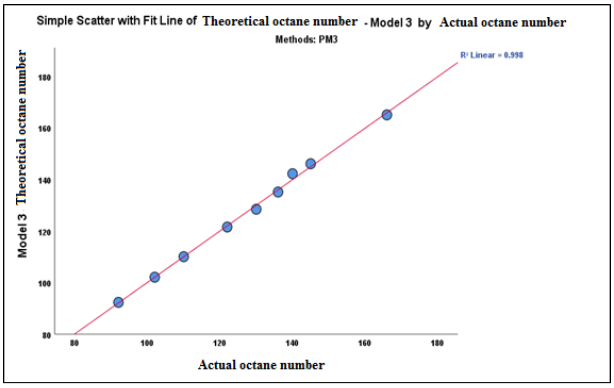


Figure 4. Simple Scatter plot with fit line for model 3

2. Conclusion

From the study of the research compounds, there is a large correspondence between the results of the practical values found in the literature and the values calculated theoretically, and this is evidence of the accuracy of the variables used in the calculations for some petroleum derivatives[12]. The best variables that influence the theoretical octane number (ON) values were HOMO and LOMO according to statistical analysis.

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