Malaya Journal of Matematik, Vol. 8, No. 1, 104-116, 2020

https://doi.org/10.26637/MJM0504/0018

Predicting physico-chemical properties of octane isomers using QSPR approach

M.C. Shanmukha[1], N.S. Basavarajappa[2]* and K.N. Anilkumar[3]

Abstract

Topological indices are very important parameters in the QSPR study. In this paper a novel topological index named as RS_2- index has been introduced. Further, we carry QSPR analysis for the set of octane isomers. The QSPR study reveals that the performance of RS_2- index is better than the $M_1(G), M_2(G), \overline{M_1}(G)$ and $\overline{M_2}(G)$.

Keywords

Topological indices, QSPR-analysis, octane isomers.

AMS Subject Classification

05C90, 05C35, 05C12.

[1] *Department of Mathematics, Jain Institute of Technology, Davanagere- 577003, Karnataka, India and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka.*

[2,3] *Department of Mathematics, Bapuji Institute of Engineering and Technology, Davanagere- 577004, Karnataka, India and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka.*

***Corresponding author**: [2]dr.nsbasavaraj@gmail.com; [1]mcshanmukha@gmail.com; [3]kn.anil5340@gmail.com

Article History: Received **27** October **2019**; Accepted **18** November **2019**

Contents

1. Introduction

Let $G = (V,E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m, thus $|V(G)| = n$ and $|E(G)| = m$. The degree of a vertex v, denoted by $d_G(v)$.

The complement of a graph G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are connected by an edge uv, if and only if they are not adjacent in G. Obviously, $E(G) \cup E(\overline{G}) = E(K_n)$, and $\overline{m} = |E(\overline{G})| = \frac{n(n-1)}{2} - m$. For undefined terminologies we refer the reader to [3].

There are two invariants called the first Zagreb index and second Zagreb index [1, 2, 4–6] defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v),$$

respectively.

In fact, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{uv \in E(G)} \big[d_G(u) + d_G(v)\big].$$

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Winer polynomials of certain composite graphs (see [1]) defined first Zagreb coindex and second Zagreb coindex as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} \left[d_G(u) + d_G(v)\right]$$

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u)\, d_G(v),$$

respectively.

It follows directly from the definition of second Zagreb coindex achieve its smallest possible value of zero. Therefore, throughout this paper, to avoid trivialities, we assume that the graphs considered have second Zagreb coindex value at least one.

Recently Hosamani et. al.,[9] have put forward ten novel topological index $S_2(G) = \sum_{uv \in E} d_G(u)^{|d_G(u)|} + d_G(v)^{|d_G(v)|}$. Based on this concept, here we considering the reciprocal version of $S_2(G)$. Which is defined as follows:

$$RS_2(G) = \frac{1}{\sum_{uv \in E} d_G(u)^{|d_G(u)|} + d_G(v)^{|d_G(v)|}}$$

.

2. QSPR Analysis $RS_2(G)$- Index

Now, we are interested in to check the chemical applicability of $RS_2(G)$ of molecular graph G. For this reason, we are interested to carry QSPR analysis of $RS_2(G)$ with the set of octane isomers. The following statistical models have been used for the study:

- Linear Model: $P = a(RS_2(G)) + b$
- Quadratic Model : $P = a(RS_2(G))^2 + b(RS_2(G)) + c$
- Logarithmic Model: $P = a + b\ln(RS_2(G))$

where P is a physical property, a, b and c are constants.

Here we have examined the chemical applicability of the RS_2-index and compared the values with the so called degree based topological indices, namely, first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$, first Zagreb coindex $\overline{M_1}(G)$ and second Zagreb coindex ($\overline{M_2}(G)$), for modeling ten representative physical properties [boiling points(BP), molar volumes (mv) at 20°C, molar refractions (mr) at 20°C, heats of vaporization (hv) at 25°C, surface tensions (st) 20°C and melting points (mp), acentric factor (AcentFac) and DHVAP] of octane isomers. The values are compiled in Table 1 [8].

3. Linear Regression Models

In this section we consider the linear regression models for $RS_2(G)$, $M_1(G)$, $M_2(G)$, $\overline{M_1}(G)$ and $\overline{M_2}(G)$ as follows:

$$\begin{aligned}
bp &= 106.090 + 15.401(RS_2(G)) \\
Heatsofvaporization &= -222.798 + 12.047(RS_2(G)) \\
TC &= 282.929 + 13.520(RS_2(G)) \\
PC &= 26.948 - 1.122(RS_2(G)) \\
S &= 98.878 + 13.213(RS_2(G)) \\
D &= 0.742 - 0.059(RS_2(G)) \\
Radius &= 1.403 + 0.458(RS_2(G)) \\
HVAP &= 37.829 + 1.573(RS_2(G)) \\
MV &= 160.257 + 1.649(RS_2(G)) \\
AF &= 0.283 + 0.107(RS_2(G)) \\
DHVAP &= 8.545 + 1.175(RS_2(G))
\end{aligned}$$

4. Quadratic Regression Models

In this section we consider the quadratic regression models for $RS_2(G)$, $M_1(G)$, $M_2(G)$, $\overline{M_1}(G)$ and $\overline{M_2}(G)$ as follows:

$$\begin{aligned}
bp &= 16.912(RS_2(G))^2 - 1.581(RS_2(G)) + 109.337 \\
hv &= 7.986(RS_2(G))^2 + 4.028(RS_2(G)) - 221.265 \\
tc &= 17.159(RS_2(G))^2 - 3.623(RS_2(G)) + 282.233 \\
pc &= 3.291(RS_2(G))^2 - 4.395(RS_2(G)) + 26.104 \\
s &= 25.445(RS_2(G))^2 - 12.182(RS_2(G)) + 96.539 \\
d &= -0.234(RS_2(G))^2 + 0.175(RS_2(G)) + 0.776 \\
r &= 0.147(RS_2(G))^2 + 0.310(RS_2(G)) + 1.463 \\
hvap &= -11.530(RS_2(G))^2 + 13.049(RS_2(G)) + 40.33 \\
mv &= 5.835(RS_2(G))^2 - 3.798(RS_2(G)) + 159.296 \\
af &= 0.154(RS_2(G))^2 - 0.047(RS_2(G)) + 0.274 \\
dhvap &= 0.854(RS_2(G))^2 + 0.320(RS_2(G)) + 8.607
\end{aligned}$$

5. Logarithmic Regression Models

In this section we consider the linear regression models for $RS_2(G)$, $M_1(G)$, $M_2(G)$, $\overline{M_1}(G)$ and $\overline{M_2}(G)$ as follows:

$$\begin{aligned}
bp &= 116.930 + 3.481(RS_2(G)) \\
Heatsofvaporization &= -213.886 + 3.190(RS_2(G)) \\
TC &= 293.843 + 4.566(RS_2(G)) \\
PC &= 26.410 + 0.018(RS_2(G)) \\
S &= 109.392 + 4.299(RS_2(G)) \\
D &= 0.689 - 0.027(RS_2(G)) \\
Radius &= 1.730 + 0.108(RS_2(G)) \\
HVAP &= 38.246 - 0.390(RS_2(G)) \\
MV &= 161.883 + 1.002(RS_2(G)) \\
AF &= 0..365 + 0.032(RS_2(G)) \\
DHVAP &= 9.413 + 0.310(RS_2(G))
\end{aligned}$$

6. Results and Discussions

The correlation coefficient(r) values for the above mentioned physical properties of octane isomers with $RS_2(G)$-index gives interesting results. Start from the linear regression models, The r values ranging from $0.022to0.597$, where as the r value for the quadratic regression model ranging from $0.032to0.602$ and for logarithmic regression model the range of r value is $0.036to0.687$.

The correlation coefficient(r) values for the physical properties of octane isomers with $M_1(G)$- index as follows: Start from the linear regression models, The r values ranging from $0.038to0.862$, where as the r value for the quadratic regression model ranging from $0.053to0.862$ and for logarithmic regression model the range of r value is $0.050to0.859$.

The correlation coefficient(r) values for the physical properties of octane isomers with $M_2(G)$- index as follows: Start from the linear regression models, The r values ranging from $0.014to0.902$, where as the r value for the quadratic regression model ranging from $0.042to0.902$ and for logarithmic regression model the range of r value is $0.014to0.897$.

The correlation coefficient(r) values for the physical properties of octane isomers with $\overline{M_1}(G)$- index as follows: Start from the linear regression models, The r values ranging from $0.038to0.862$, where as the r value for the quadratic regression model ranging from $0.029to0.861$ and for logarithmic regression model the range of r value is $0.053to0.862$.

The correlation coefficient(r) values for the physical properties of octane isomers with $\overline{M_2}(G)$- index as follows: Start from the linear regression models, The r values ranging from $0.027to0.848$, where as the r value for the quadratic regression model ranging from $0.031to0.862$ and for logarithmic regression model the range of r value is $0.043to0.865$.

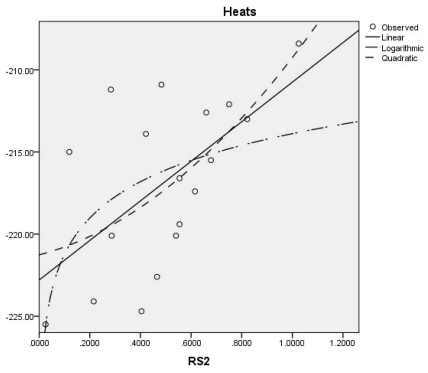
For model (1), the $RS_2(G)$- index shows minimum correlation with molar volume and the maximum correlation with the DHVAP of the octane isomers, the $M_1(G)$ shows minimum correlation with HVAP and the maximum correlation with AF, the the $M_2(G)$ shows minimum correlation with HVAP and the maximum correlation with AF, the $\overline{M_1}(G)$ shows minimum correlation with HVAP and the maximum correlation with AF and finally the $\overline{M_2}(G)$ shows minimum correlation with HVAP and the maximum correlation with entropy.

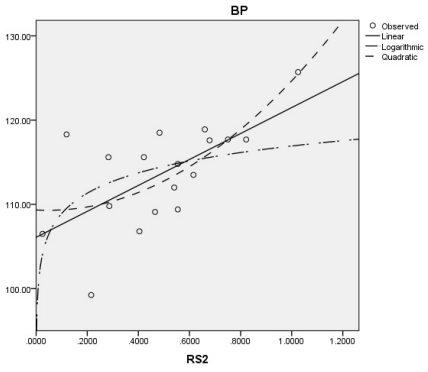
For model (2), the $RS_2(G)$- index shows minimum correlation with molar volume and the maximum correlation with the DHVAP of the octane isomers, the $M_1(G)$ shows minimum correlation with MV and the maximum correlation with AF, the the $M_2(G)$ shows minimum correlation with TC and the maximum correlation with AF, the $\overline{M_1}(G)$ shows minimum correlation with HVAP and the maximum correlation with AF and finally the $\overline{M_2}(G)$ shows minimum correlation with TC and the maximum correlation with entropy.

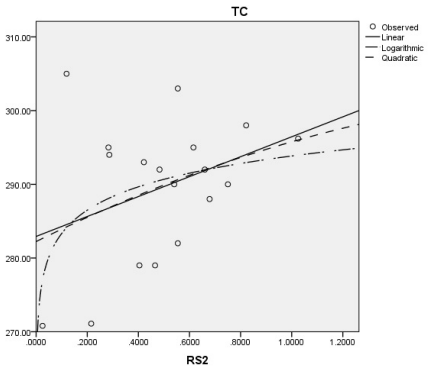
Finally, for model (3), the $RS_2(G)$- index shows minimum correlation with HVAP and the maximum correlation with the D of the octane isomers, the $M_1(G)$ shows minimum correlation with MV and the maximum correlation with AF, the the $M_2(G)$ shows minimum correlation with TC and the maximum correlation with AF, the $\overline{M_1}(G)$ shows minimum correlation with MV and the maximum correlation with AF and finally the $\overline{M_2}(G)$ shows minimum correlation with TC and the maximum correlation with entropy.

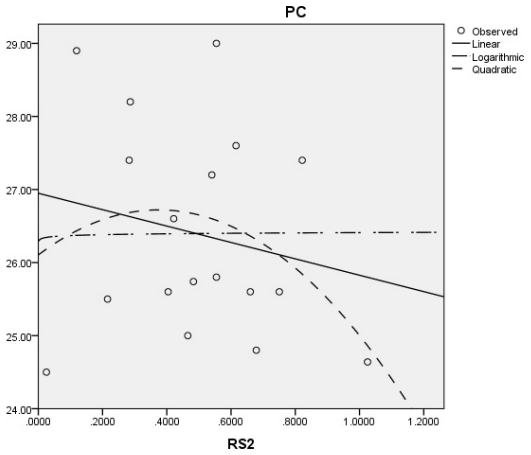
7. The Correlations of $RS_1(G)$ with the Physico-chemical Properties of Octane isomers

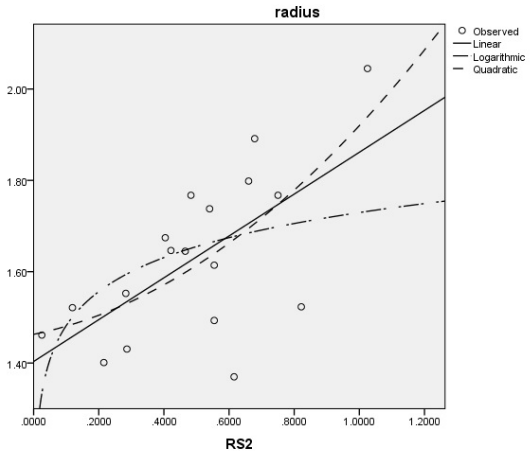
The correlation coefficient of $RS_2(G)$ with above mentioned physical properties are depicted in the following figures.

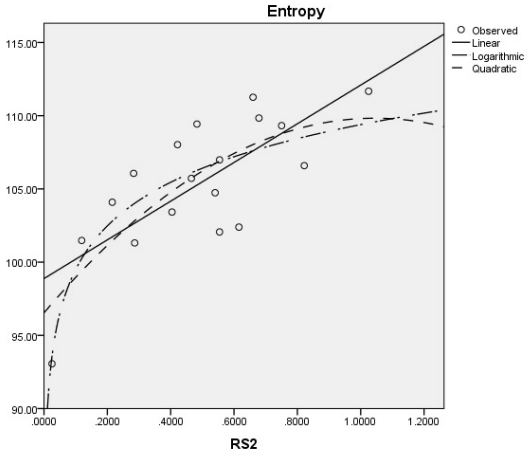


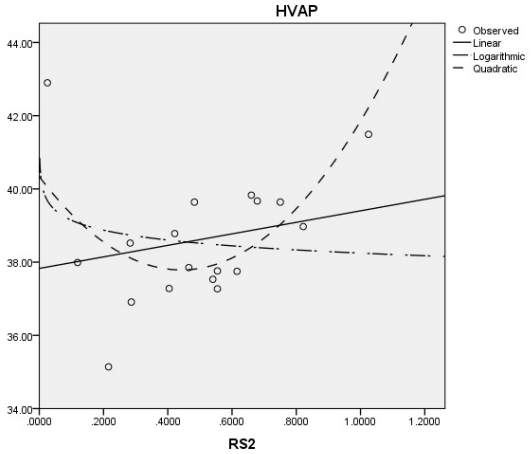


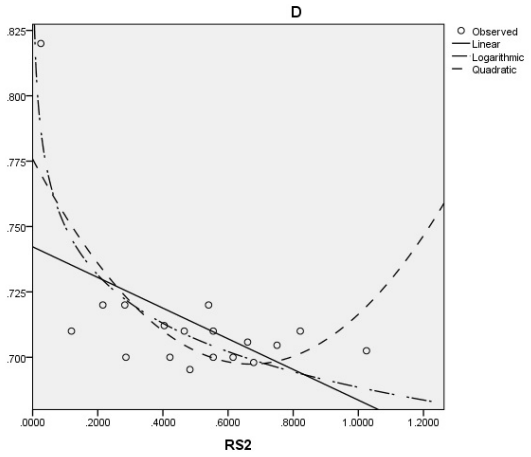


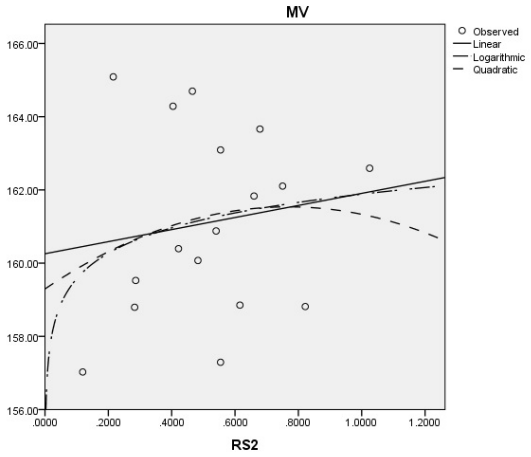

PC
Observed
Linear
Logarithmic
Quadratic
29.00
28.00
27.00
26.00
25.00
24.00
.0000
.2000
.4000
.6000
.8000
1.0000
1.2000
RS2

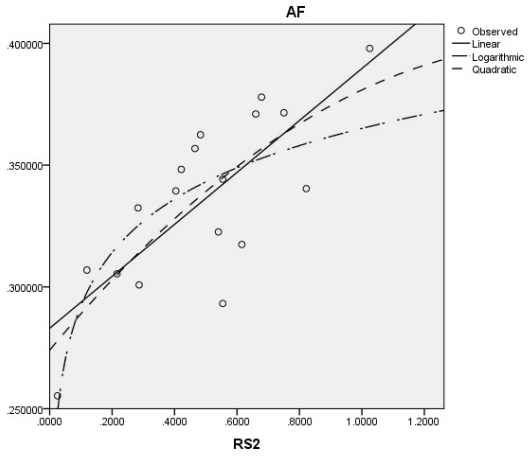

radius
Observed
Linear
Logarithmic
Quadratic
2.00
1.80
1.60
1.40
.0000
.2000
.4000
.6000
.8000
1.0000
1.2000
RS2

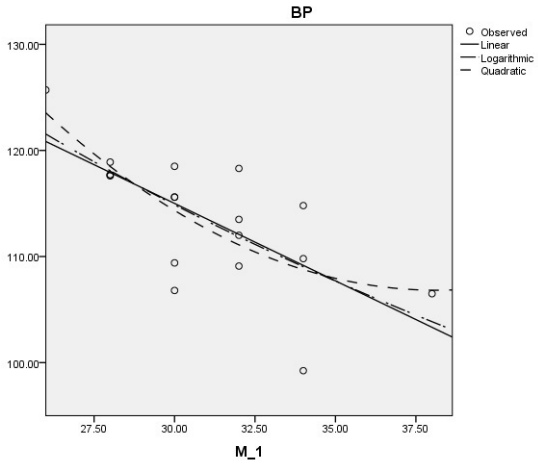

Entropy
Observed
Linear
Logarithmic
Quadratic
115.00
110.00
105.00
100.00
95.00
90.00
.0000
.2000
.4000
.6000
.8000
1.0000
1.2000
RS2

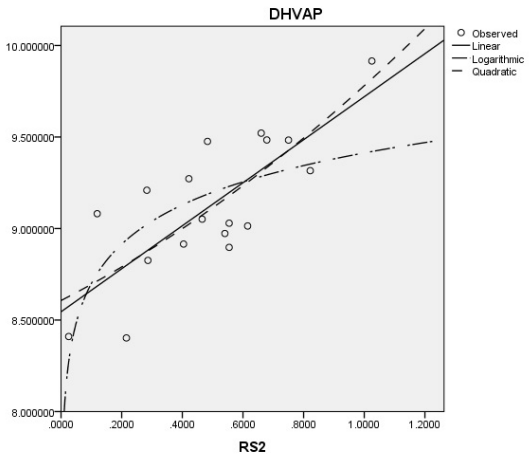

HVAP
Observed
Linear
Logarithmic
Quadratic
44.00
42.00
40.00
38.00
36.00
34.00
.0000
.2000
.4000
.6000
.8000
1.0000
1.2000
RS2

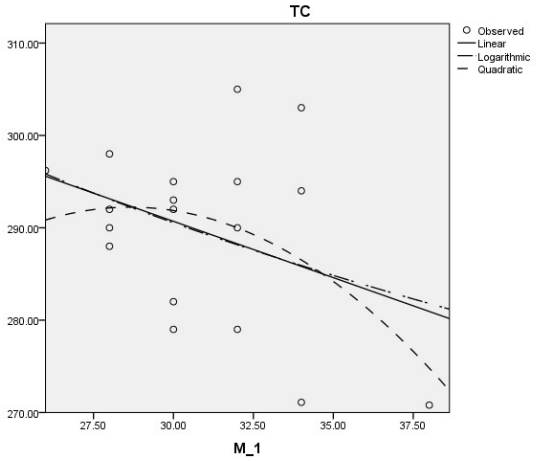

D
Observed
Linear
Logarithmic
Quadratic
.825
.800
.775
.750
.725
.700
.0000
.2000
.4000
.6000
.8000
1.0000
1.2000
RS2

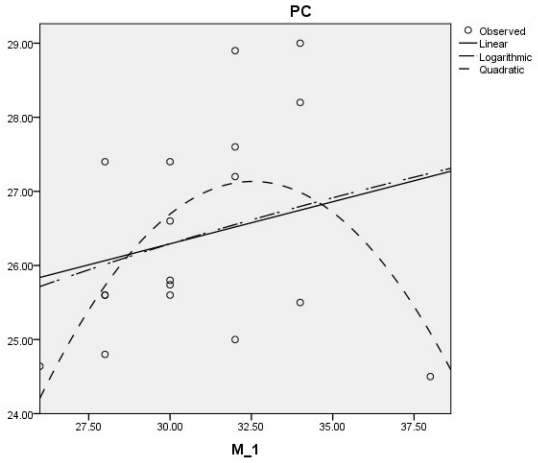

MV
Observed
Linear
Logarithmic
Quadratic
166.00
164.00
162.00
160.00
158.00
156.00
.0000
.2000
.4000
.6000
.8000
1.0000
1.2000
RS2





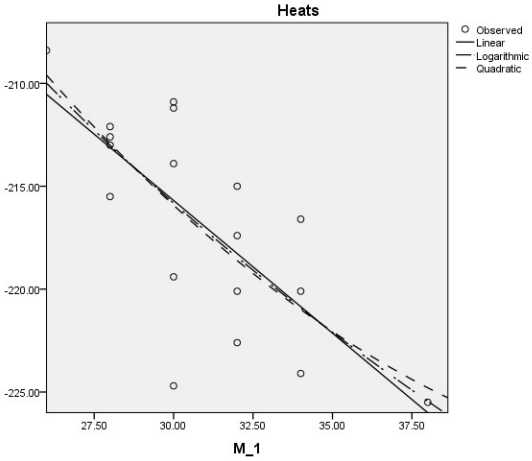


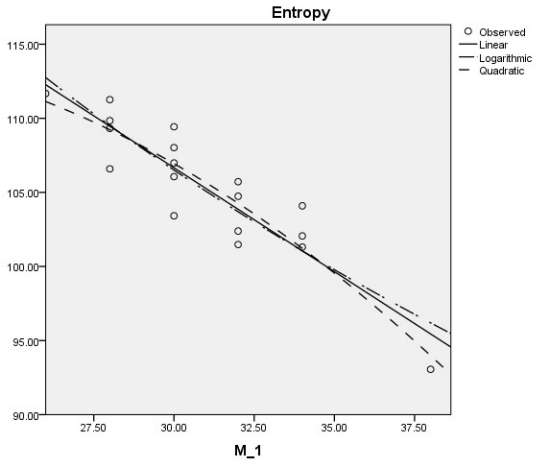


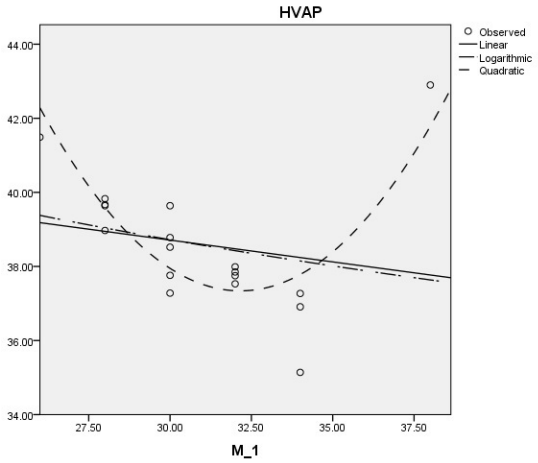


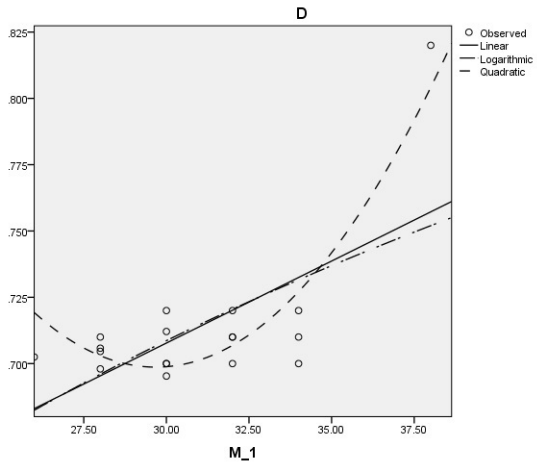
8. The Correlations of $M_1(G)$ with the Physico-chemical Properties of Octane isomers

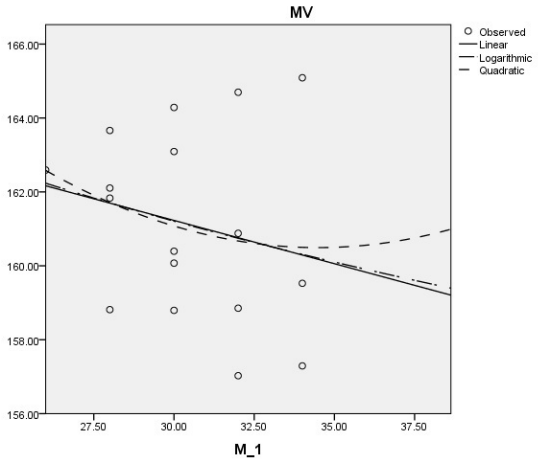
The correlation coefficient of $M1(G)$ with above mentioned physical properties are depicted in the following figures.

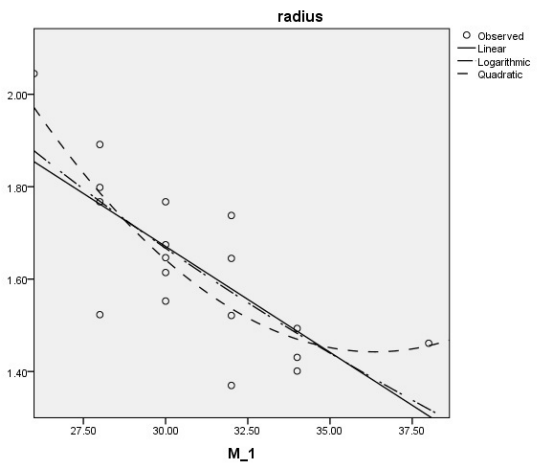


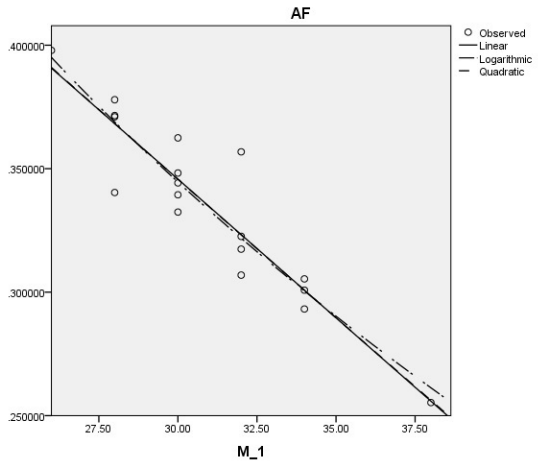

Entropy
Observed
Linear
Logarithmic
Quadratic
115.00
110.00
105.00
100.00
95.00
90.00
27.50
30.00
32.50
35.00
37.50
M_1

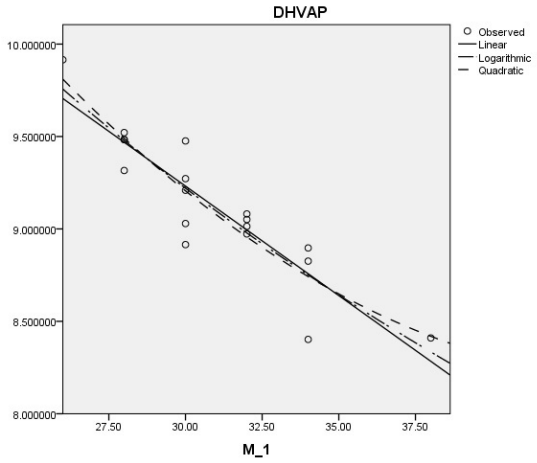

HVAP
Observed
Linear
Logarithmic
Quadratic
44.00
42.00
40.00
38.00
36.00
34.00
27.50
30.00
32.50
35.00
37.50
M_1

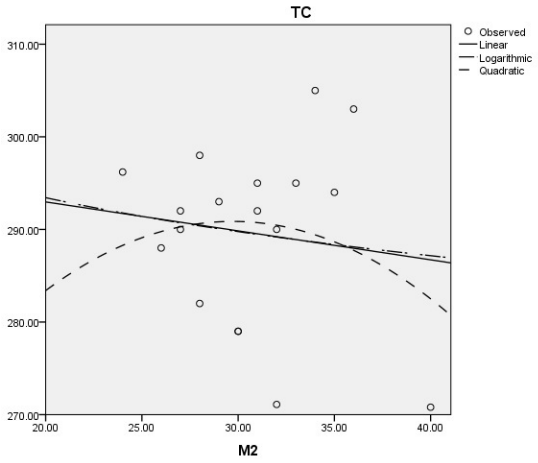

D
Observed
Linear
Logarithmic
Quadratic
.825
.800
.775
.750
.725
.700
27.50
30.00
32.50
35.00
37.50
M_1


MV
Observed
Linear
Logarithmic
Quadratic
166.00
164.00
162.00
160.00
158.00
156.00
27.50
30.00
32.50
35.00
37.50
M_1


radius
Observed
Linear
Logarithmic
Quadratic
2.00
1.80
1.60
1.40
27.50
30.00
32.50
35.00
37.50
M_1

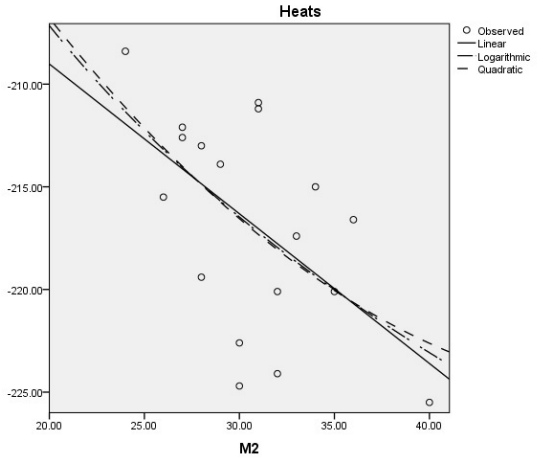

AF
Observed
Linear
Logarithmic
Quadratic
.400000
.350000
.300000
.250000
27.50
30.00
32.50
35.00
37.50
M_1

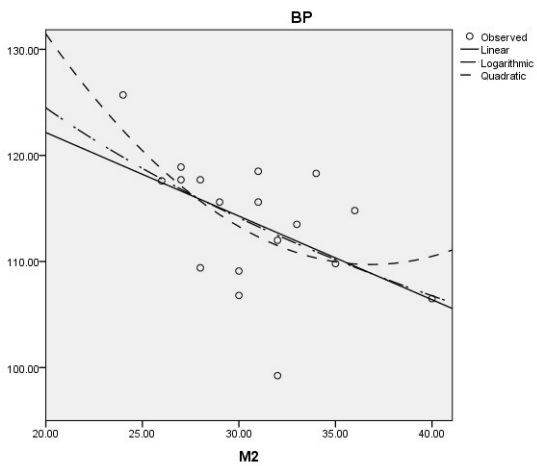


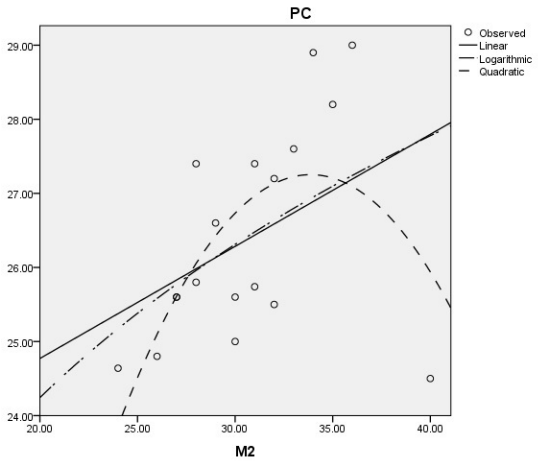


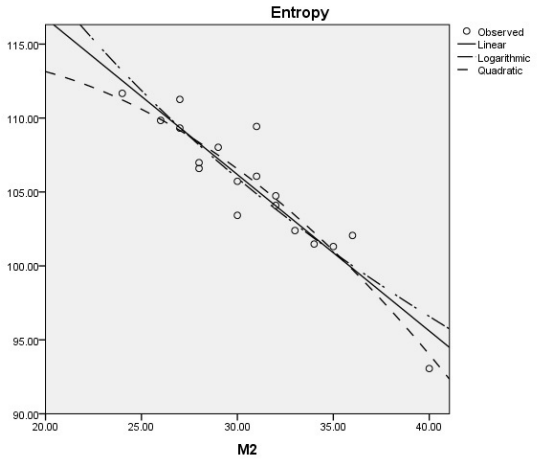
9. The Correlations of $M_2(G)$ with the Physico-chemical Properties of Octane isomers

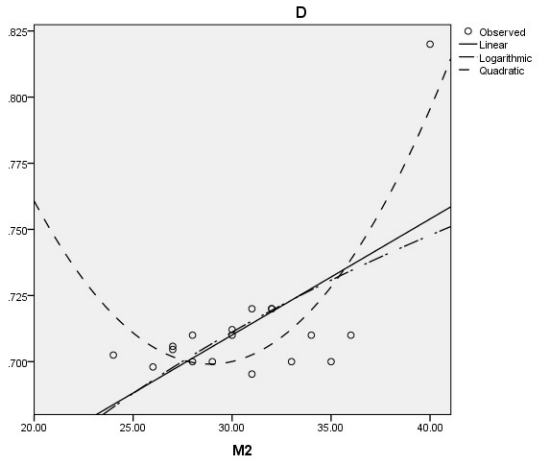
The correlation coefficient of $M2(G)$ with above mentioned physical properties are depicted in the following figures.

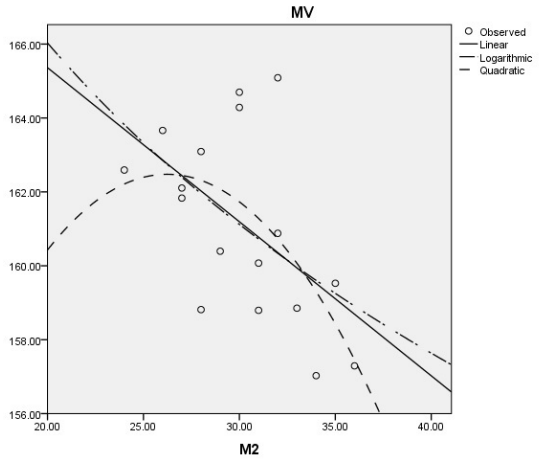


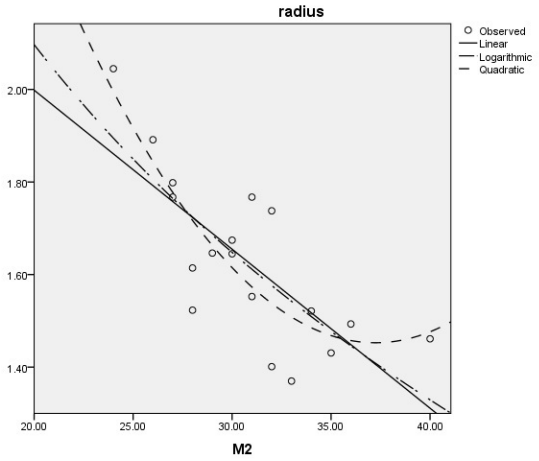


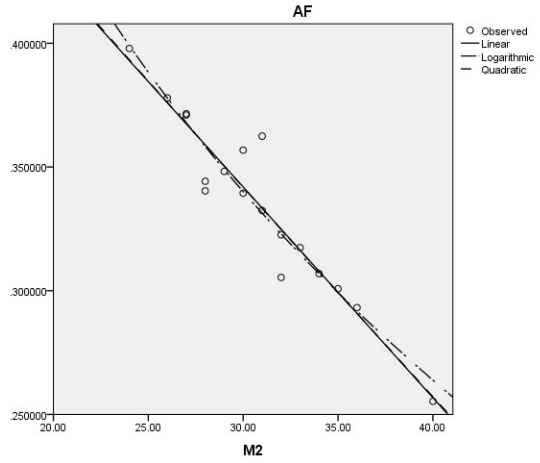


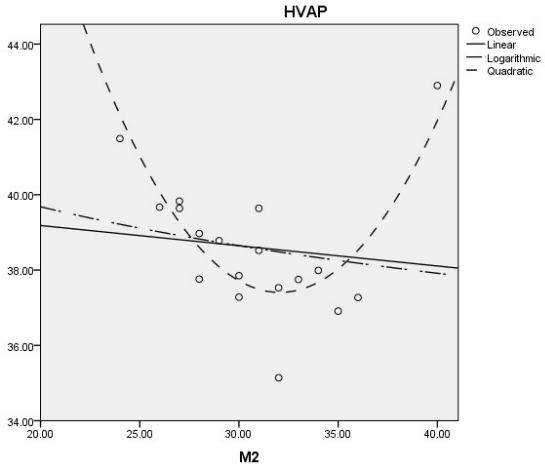


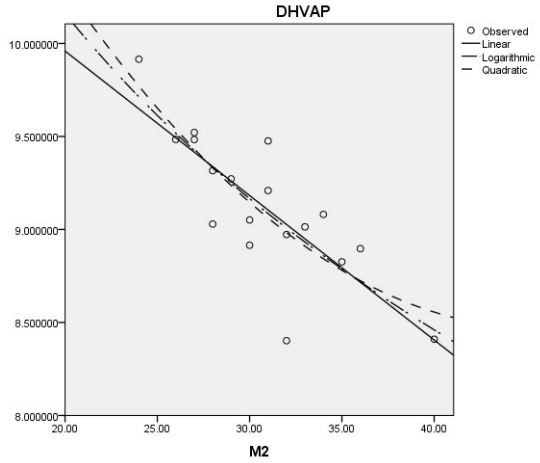






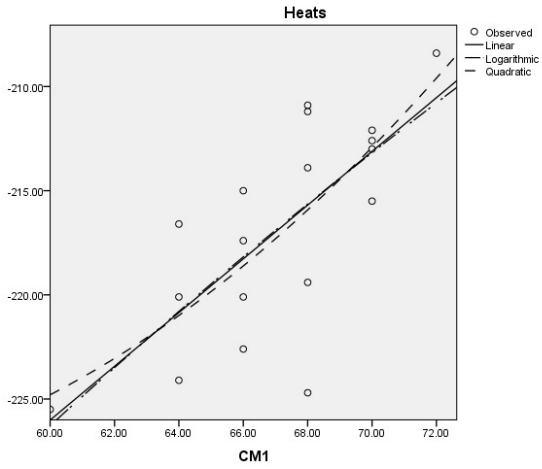


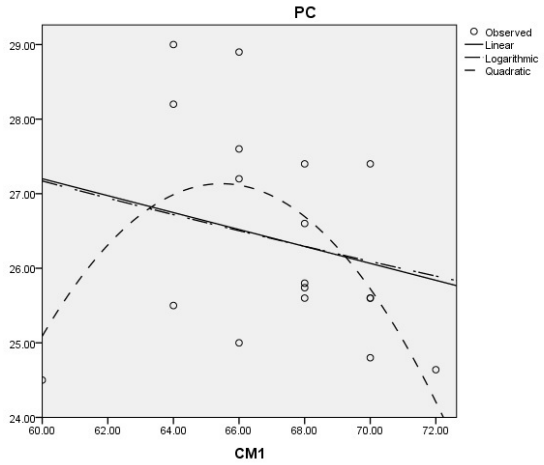


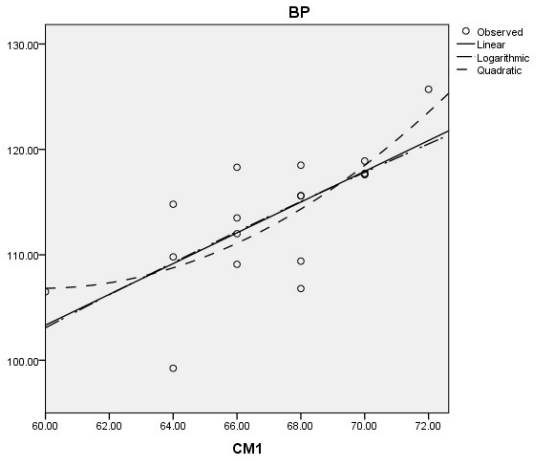


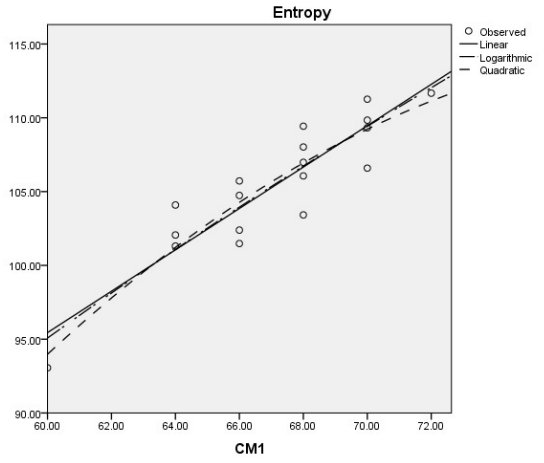
10. The Correlations of $\overline{M_1}(G)$ with the Physico-chemical Properties of Octane isomers

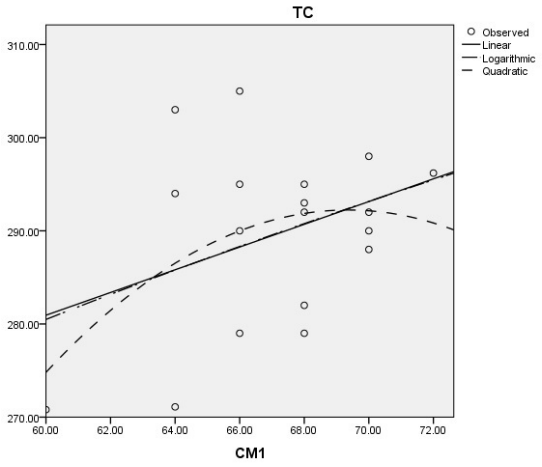
The correlation coefficient of $\overline{M1}(G)$ with above mentioned physical properties are depicted in the following figures.

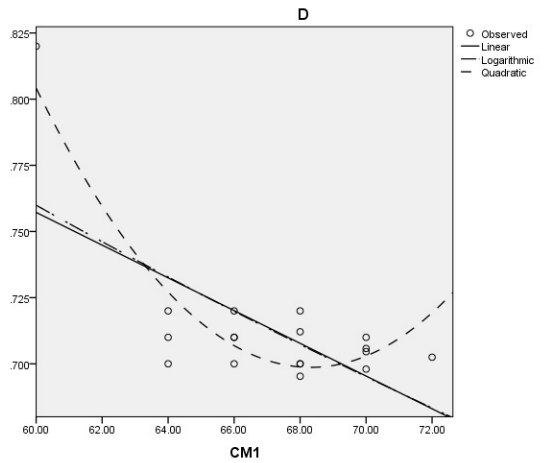

Heats
Observed
Linear
Logarithmic
Quadratic
-210.00
-215.00
-220.00
-225.00
60.00
62.00
64.00
66.00
68.00
70.00
72.00
CM1

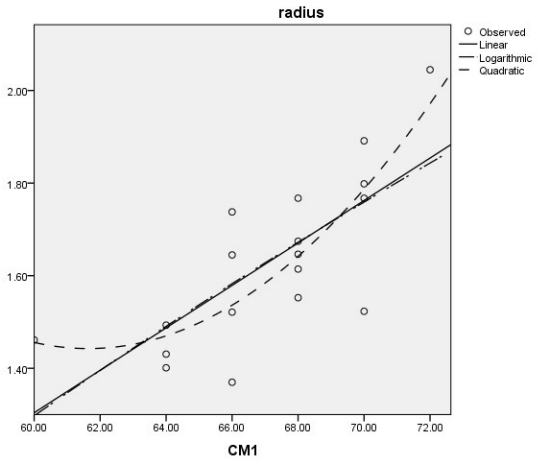

PC
Observed
Linear
Logarithmic
Quadratic
29.00
28.00
27.00
26.00
25.00
24.00
60.00
62.00
64.00
66.00
68.00
70.00
72.00
CM1

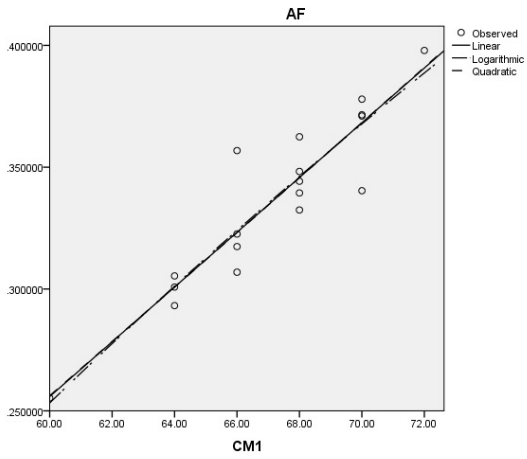

BP
Observed
Linear
Logarithmic
Quadratic
130.00
120.00
110.00
100.00
60.00
62.00
64.00
66.00
68.00
70.00
72.00
CM1

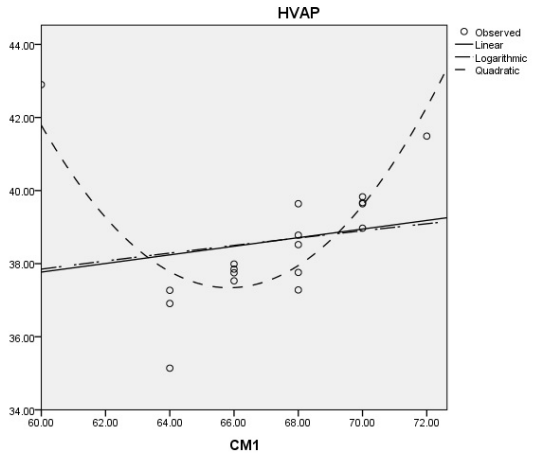

Entropy
Observed
Linear
Logarithmic
Quadratic
115.00
110.00
105.00
100.00
95.00
90.00
60.00
62.00
64.00
66.00
68.00
70.00
72.00
CM1

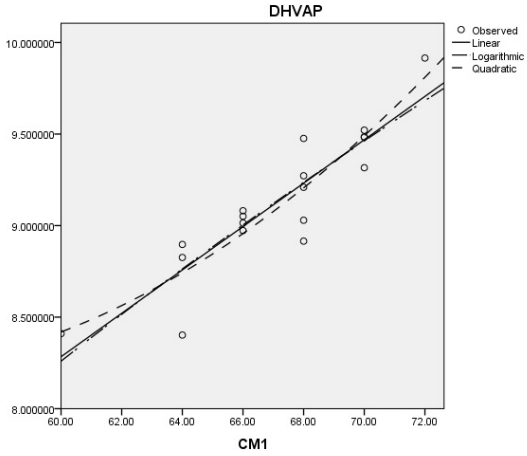

TC
Observed
Linear
Logarithmic
Quadratic
310.00
300.00
290.00
280.00
270.00
60.00
62.00
64.00
66.00
68.00
70.00
72.00
CM1

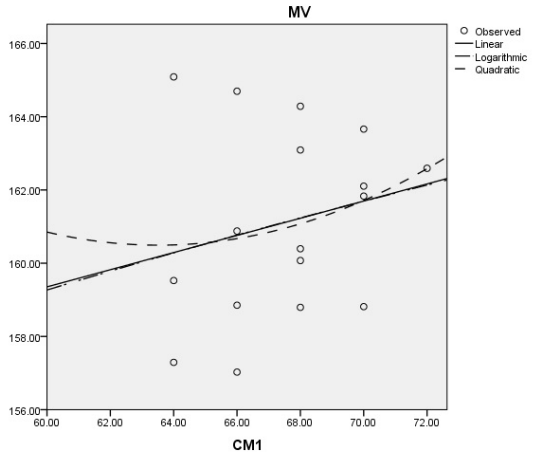

D
Observed
Linear
Logarithmic
Quadratic
.825
.800
.775
.750
.725
.700
60.00
62.00
64.00
66.00
68.00
70.00
72.00
CM1





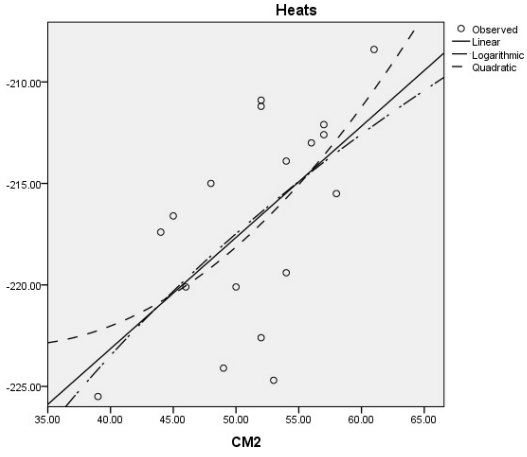


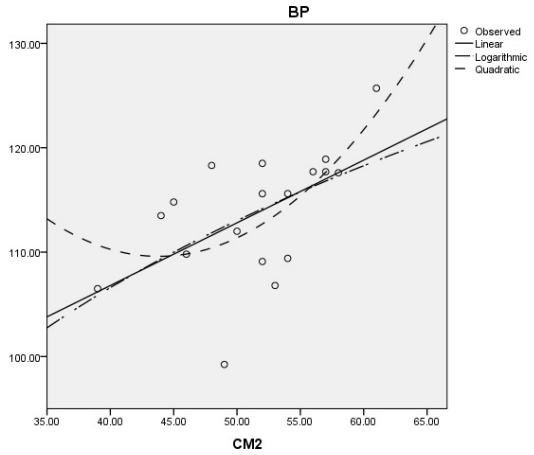


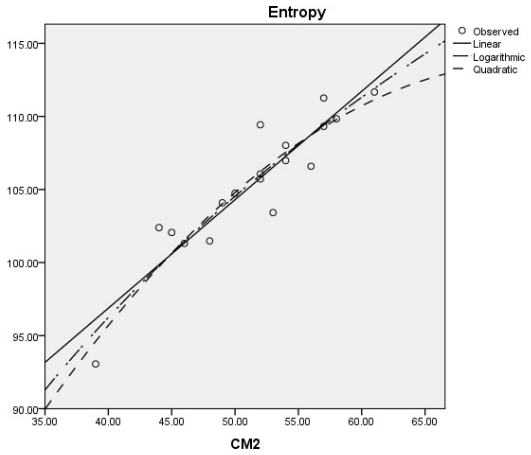


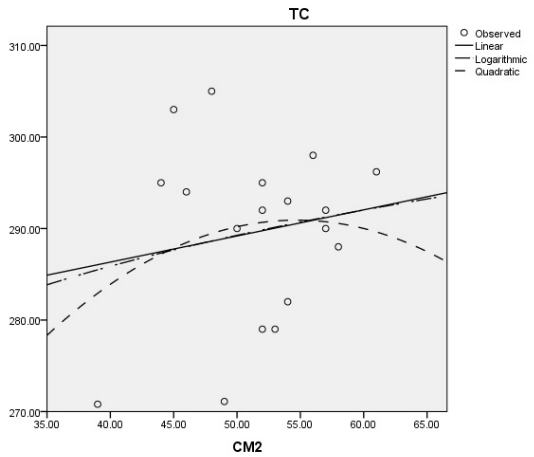
11. The Correlations of $\overline{M_2}(G)$ with the Physico-chemical Properties of Octane isomers

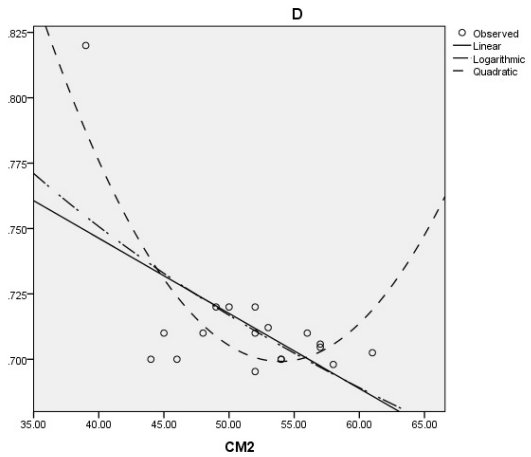
The correlation coefficient of $\overline{M2}(G)$ with above mentioned physical properties are depicted in the following figures.

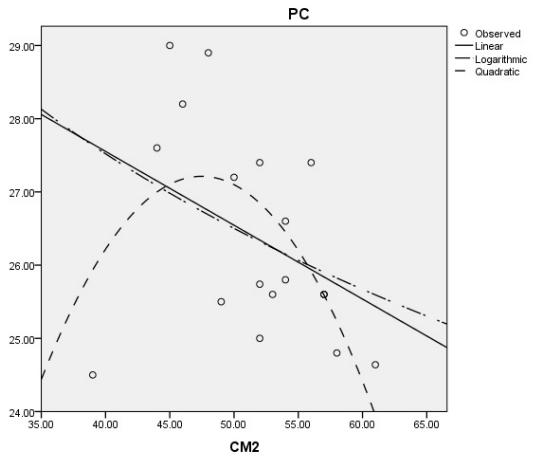


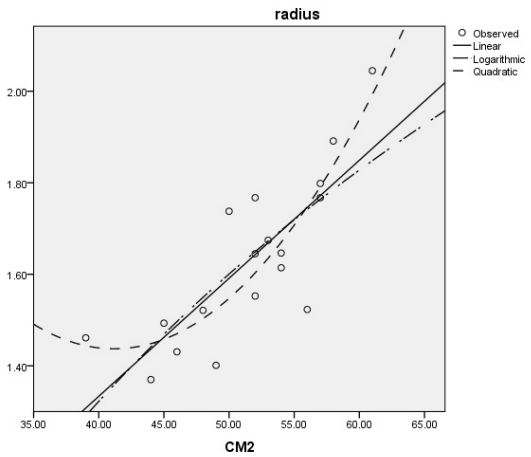

BP
Observed
Linear
Logarithmic
Quadratic
130.00
120.00
110.00
100.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
CM2

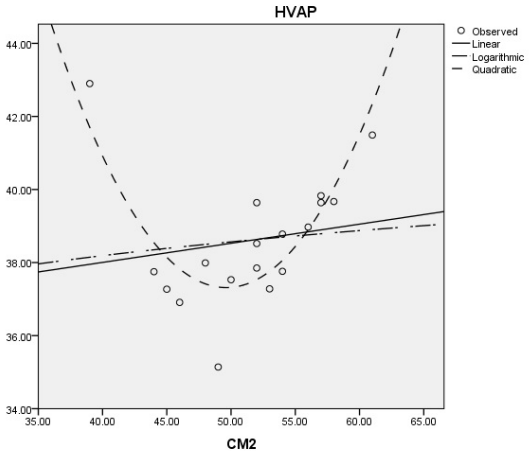

Entropy
Observed
Linear
Logarithmic
Quadratic
115.00
110.00
105.00
100.00
95.00
90.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
CM2

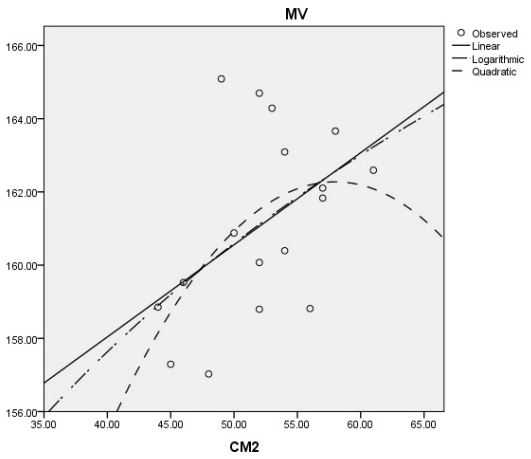

TC
Observed
Linear
Logarithmic
Quadratic
310.00
300.00
290.00
280.00
270.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
CM2

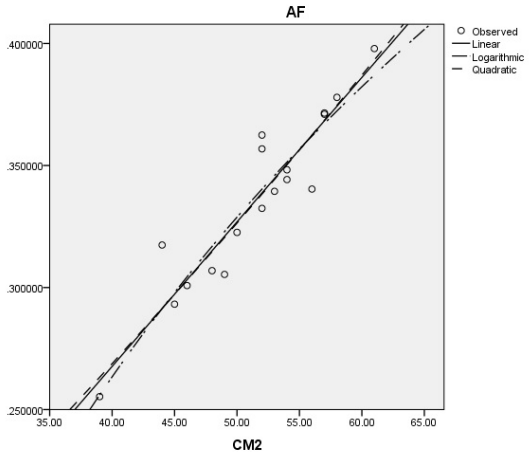

D
Observed
Linear
Logarithmic
Quadratic
.825
.800
.775
.750
.725
.700
35.00
40.00
45.00
50.00
55.00
60.00
65.00
CM2

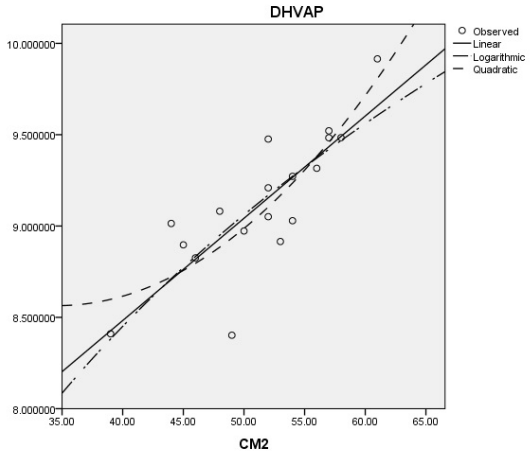

PC
Observed
Linear
Logarithmic
Quadratic
29.00
28.00
27.00
26.00
25.00
24.00
35.00
40.00
45.00
50.00
55.00
60.00
65.00
CM2


radius
Observed
Linear
Logarithmic
Quadratic
2.00
1.80
1.60
1.40
35.00
40.00
45.00
50.00
55.00
60.00
65.00
CM2









12. Conclusion

The results of QSPR studies reveals that the regression models (1)-(3) are the most significant models to predict the physicochemical properties of molecular graphs.

13. Acknowledgment

The authors are thankful to the anonymous reviewers for their useful comments to improve the quality of the paper.

References

[1] A. R. Ashrafi, T. Došlić, A. Hamzeh, The Zagreb coindices of graph operations, *Discrete Appl. Math.* 158 (2010) 1571-1578.

[2] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* 86(4)(2013) 351-361.

[3] F. Harary, *Graph Theory*, Addison–Wesely, Reading, 1969.

[4] S. M. Hosamani, I. Gutman, Zagreb indices of transformation and total transformation graphs, *Appl. Math.Comput.,* 247 (2014), 1156–1160.

[5] S. M. Hosamani, B. Basavanagoud, New upper bounds for the first Zagreb index, *MATCH Commun. Math. Comput. Chem.,* 74(1)(2015), 97–101.

[6] S. M. Hosamani, S. H. Malghan and I. N. Cangul, The first geometric-arithmetic index of graph operations, *Advances and Applications in Mathematical Sciences*, 14(6)(2015), 155–163.

[7] S. M. Hosamani, Computing Sanskruti index of certain nanostructures, *J. Appl. Math. Comput.,* 1-9 (2016) DOI 10.1007/s12190-016-1016-9.

[8] S. M. Hosamani Correlation of domination parameters with physicochemical properties of octane isomers. *Applied Mathematics and Nonlinear Sciences*, 1(2016), 345–352.

[9] S. M. Hosamani, V.B. Awati and R. M. Honnamore, Estimation of numerical invariants associated with certain

nanostructures and dendrimers via degree based descriptors, *Journal of Mathemaical Chemistry,* (Accepted).

[10] M. Thakur, A. Thakur, P.V. Khadikar, QSAR study of benzene sulphonamadie carbonic anhydrase inhibitors: Topological approach using Balban index, *Bioorg. Med. Chem.,* 12(4)(2004), 789–793.

[11] N. Trinajstić, Chemical graph theory, *CRC Press,* 1992.

⋆⋆⋆⋆⋆⋆⋆⋆⋆
ISSN(P):2319 – 3786
Malaya Journal of Matematik
ISSN(O):2321 – 5666
⋆⋆⋆⋆⋆⋆⋆⋆⋆