International Journal of Science and Research (IJSR)
ISSN: 2319-7064
SJIF (2022): 7.942

Mean Zagreb Index and Its Applications to Chemical Networks

Vidya S. Umadi[a] and A. M. Sangogi[b]

[a]*Department of Mathematics, Vidya Samvardhak Mandal's Somashekhar R.Kothiwale Institute of Technology, Nipani, Karnataka State, India*
e-mail[a]: vidyaumadi@gmail.com
[b]*Department of Mathematics, Shaikh College of Engineering and Technology Belagavi, Karnataka State, India*

Abstract

The Zagreb indices plays vital role in chemical graph theory. In this paper we put forward a new variations of Zagreb indices, we call it as the mean Zagreb Indices. Further, we show that these parameters are highly correlated with physical properties of octane isomers. Finally we carry out QSPR (Quantitative Structure-Property Relationship) analysis using several physicochemical properties of octane isomers.

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 $|E(G)| = m$. For undefined terminologies we refer the reader to [8].

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are also called topological indices. Hundreds of different invariants have been employed to date (with unequal success) in QSAR/QSPR studies. Among more useful of them appear two that are known under various names, but mostly as Zagreb indices. Due to their chemical relevance they have been subject of numerous papers in chemical literature. There are two invariants called the first Zagreb index and second Zagreb index [1, 2, 5–7, 9–12, 14], defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v),$$

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

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} \big[d_G(u) + d_G(v)\big] \qquad \text{and} \qquad \overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u)\, d_G(v),$$

respectively.

The Forgotten Topological Index [4] is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3. \tag{1}$$

Miličević et. al [13] reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees:

$$EM_1(G) = \sum_{e \in E(G)} d_G(e)^2 \qquad \text{and} \qquad EM_2(G) = \sum_{e \sim f \in E(G)} d_G(e)\, d_G(f),$$

where $d_G(e)$ denotes the degree of an edge $e = uv$ in G, which is defined by $d_G(e) = d_G(u) + d_G(v) - 2$ and $e \sim f$ means that the edges e and f are adjacent.

Noticing that contribution of nonadjacent edges pairs should be taken into account, the reformulated Zagreb coindices can be defined as:

$$\overline{EM_1}(G) = \sum_{e \nsim f \notin E(G)} \big[d_G(e) + d_G(f)\big] \qquad \text{and} \qquad \overline{EM_2}(G) = \sum_{e \nsim f \notin E(G)} d_G(e)\, d_G(f),$$

where $d_G(e)$ denotes the degree of an edge $e = uv$ in $J(G)$, which is defined by $d_{J(G)}(e) = m + 1 - (d_G(u) + d_G(v))$ and $e \nsim f$ means that the edges e and f are non adjacent.

We define a new degree invariant and call it as the mean degree of a vertex $v \in V(G)$. Which is defined as $deg_a(v) = \frac{\sum_{u \sim v} deg(u)}{|deg(v)|}$.

Motivated by the earlier research on topological indices, here we conceive a new degree based topological index in terms of mean degree of a vertex, we call it as the first mean Zagreb index and is is defined as follows:

$$M_1^a(G) = \sum_{u \in V(G)} deg_a(u)^2. \tag{2}$$

To illustrate our concept, consider the graph G which is depicted in Fig.1.

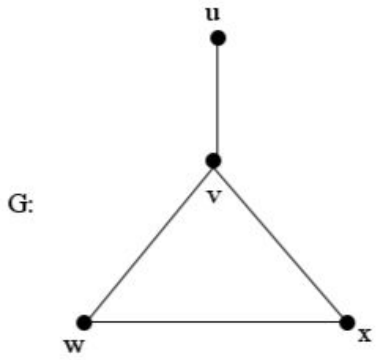


Figure 1.

The mean degrees of each vertex in G is given by

$$deg_a(u) = \frac{3}{1} = 3;\ deg_a(v) = \frac{1+2+2}{3} = \frac{5}{3};$$

$$deg_a(w) = deg_a(x) = \frac{3+2}{2} = \frac{5}{2};$$

Therefore, the the first mean Zagreb index is $M_1^a(G) = 18.0277$.

2 QSPR Analysis of the First Average Zagreb Index

Here we have examined the chemical applicability of the first mean Zagreb 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 $\overline{M_1(G)}$, second Zagreb coindex $(\overline{M_2(G)})$, Forgotten index $F(G)$, first reformulated Zagreb index $EM_1(G)$, second reformulated Zagreb index $EM_2(G)$, first reformulated Zagreb coindex $\overline{EM_1(G)}$, second reformulated 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 $M_1^a(G)$ was tested using a data set of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm.

3 Data based and analytical method

Eight physicochemical properties of octane isomers have been selected on the availability [15] of a suitable body of data: boiling point (BP), critical temperature (CT), critical

pressure (CP), entropy (S), density (D), mean radius (R_m^2) and heat of vaporization (H_v), heat of formation (H_f). The values are compiled in Table 1.

Table 1- Physico-chemical properties of octane isomers

Alkane	AF	DHVAP	BP	TC	PC	S	D	R_m^2	$-\Delta H_f$	$-\Delta H_v$
n-octane	0.397898	9.915	125.70	296.20	24.64	111.67	0.7025	2.0449	208.6	41.49
2M	0.377916	9.484	117.6	288.0	24.80	109.84	0.6980	1.8913	215.4	39.67
3M	0.371002	9.521	118.9	292.0	25.60	111.26	0.7058	1.7984	212.5	39.83
4M	0.371504	9.483	117.7	290.0	25.60	109.32	0.7046	1.7673	210.7	39.64
3E	0.362472	9.476	118.5	292.0	25.74	109.43	0.7136	1.7673	210.7	39.64
22MM	0.339426	8.915	106.8	279.0	25.60	103.42	0.6953	1.6744	224.6	37.28
23MM	0.348247	9.272	115.6	293.0	26.60	108.02	0.7121	1.6464	213.8	38.78
24MM	0.344223	9.029	109.4	282.0	25.80	106.98	0.7004	1.6142	219.2	37.76
25MM	0.35683	9.051	109.1	279.0	25.00	105.72	0.6935	1.6449	222.5	37.85
33MM	0.322596	8.973	112.0	290.8	27.20	104.74	0.7100	1.7377	220.0	37.53
34MM	0.340345	9.316	117.7	298.0	27.40	106.59	0.7200	1.5230	212.8	38.97
2M3E	0.332433	9.209	115.6	295.0	27.40	106.06	0.7193	1.5525	211.0	38.52
3M3E	0.306899	9.081	118.3	305.0	28.90	101.48	0.7274	1.5212	214.8	37.99
223MMM	0.300816	8.826	109.8	294.0	28.20	101.31	0.7161	1.4306	220.0	36.91
224MMM	0.30537	8.402	99.24	271.1	25.50	104.09	0.6919	1.4010	224.0	35.14
233MM	0.293177	8.897	114.8	303.0	29.00	102.06	0.7262	1.4931	216.3	37.27
234MMM	0.317422	9.014	113.5	295.0	27.60	102.39	0.7191	1.3698	217.3	37.75
2233MMMM	0.255294	8.41	106.5	270.8	24.50	93.06	0.8242	1.4612	225.6	42.90

The correlation of above mentioned degree based topological indices with physicochemical properties of octane isomers are given in table 2.

Table 2- Correlation of degree based topological indices with physicochemical properties of octane isomers

	AF	DHVAP	BP	TC	PC	S	D	R_m^2	ΔH_f	ΔH_v
M_1^a	0.831	0.849	0.701	0.473	0.042	0.810	0.636	0.687	0.107	0.027
M_1	0.928	.905	0.727	0.698	0.231	0.909	0.653	0.742	0.194	0.220
M_2	0.950	0.801	0.509	0.127	0.416	0.925	0.625	0.750	0.120	0.540
$\overline{M_1}$	0.928	0.905	0.698	0.367	0.231	0.909	0.653	0.742	0.194	0.220
$\overline{M_2}$	0.936	0.819	0.550	0.164	0.393	0.921	0.581	0.799	0.165	0.474
F	0.919	0.892	0.679	0.366	0.214	0.906	0.673	0.707	0.167	0.207
EM_1	0.941	0.853	0.597	0.259	0.300	0.927	0.675	0.714	0.128	0.365
EM_2	0.949	0.820	0.534	0.213	0.312	0.927	0.710	0.676	0.0058	0.447
$\overline{EM_1}$	0.063	0.306	0.441	0.461	0.308	0.093	0.030	0.088	0.204	0.482
$\overline{EM_2}$	0.579	0.780	0.815	0.730	0.253	0.524	0.554	0.580	0.163	0.4170

4 Results and Discussion

From table 2, it is found that the correlation coefficient of the degree based topological indices with physicochemical properties of isomers are found to be good except critical

pressure heats of vaporization and heats of formation.

A generalized linear regression model has been proposed for the relationship of physicochemical properties of octane isomers with the $M_1^a(G)$, $M_1(G)$, $M_2(G)$, $\overline{M_1}(G)$, $\overline{M_2}(G)$, $F(G)$, $EM_1(G)$, $EM_2(G)$, $\overline{EM_1}(G)$ and $\overline{EM_2}(G)$ respectively.

$$P = a + \sum_{i=1}^{10} b_i X_i \tag{3}$$

where P refers to a physicochemical property, a is constant, b_i the sensitivity of X_i towards P. For our convince we assume $X_1 = M_1^a(G)$, $X_2 = M_1(G)$, $X_3 = M_2(G)$, $X_4 = \overline{M_1}(G)$, $X_5 = \overline{M_2}(G)$, $X_6 = F(G)$, $X_7 = EM_1(G)$, $X_8 = EM_2(G)$, $X_9 = \overline{EM_1}(G)$ and $X_{10} = \overline{EM_2}(G)$

We first consider the regression model containing single descriptors $M_1^a(G)$, $M_1(G)$, $M_2(G)$, $\overline{M_1}(G)$, $\overline{M_2}(G)$, $F(G)$, $EM_1(G)$, $EM_2(G)$, $\overline{EM_1}(G)$ and $\overline{EM_2}(G)$ respectively.

$$P = a + bM_1^a(G) \tag{4}$$

$$P = a + bM_1(G) \tag{5}$$

$$P = a + bM_2(G) \tag{6}$$

$$P = a + b\overline{M_1}(G) \tag{7}$$

$$P = a + b\overline{M_2}(G) \tag{8}$$

$$P = a + bF(G) \tag{9}$$

$$P = a + bEM_1(G) \tag{10}$$

$$P = a + bEM_2(G) \tag{11}$$

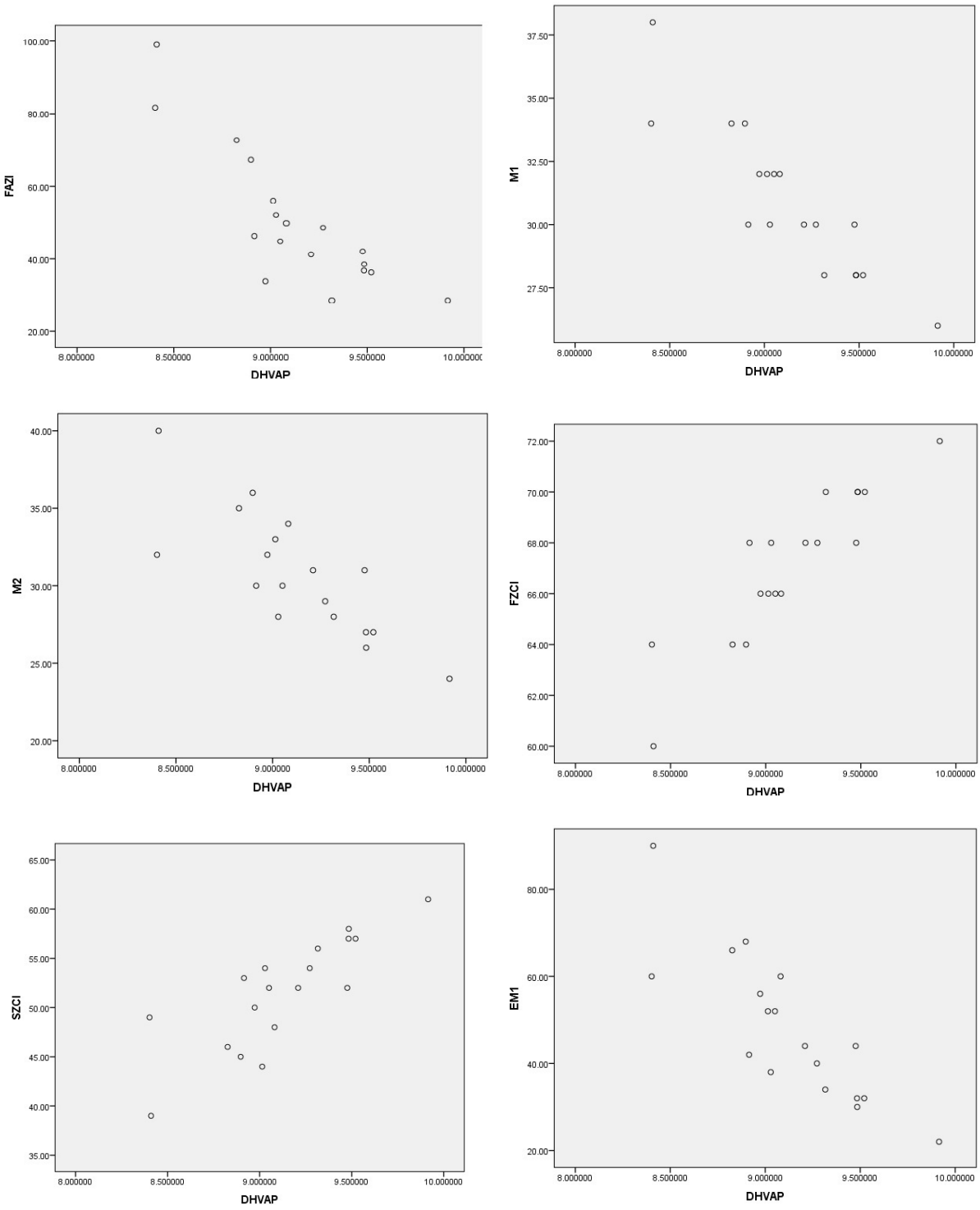
$$P = a + b\overline{EM_1}(G) \tag{12}$$

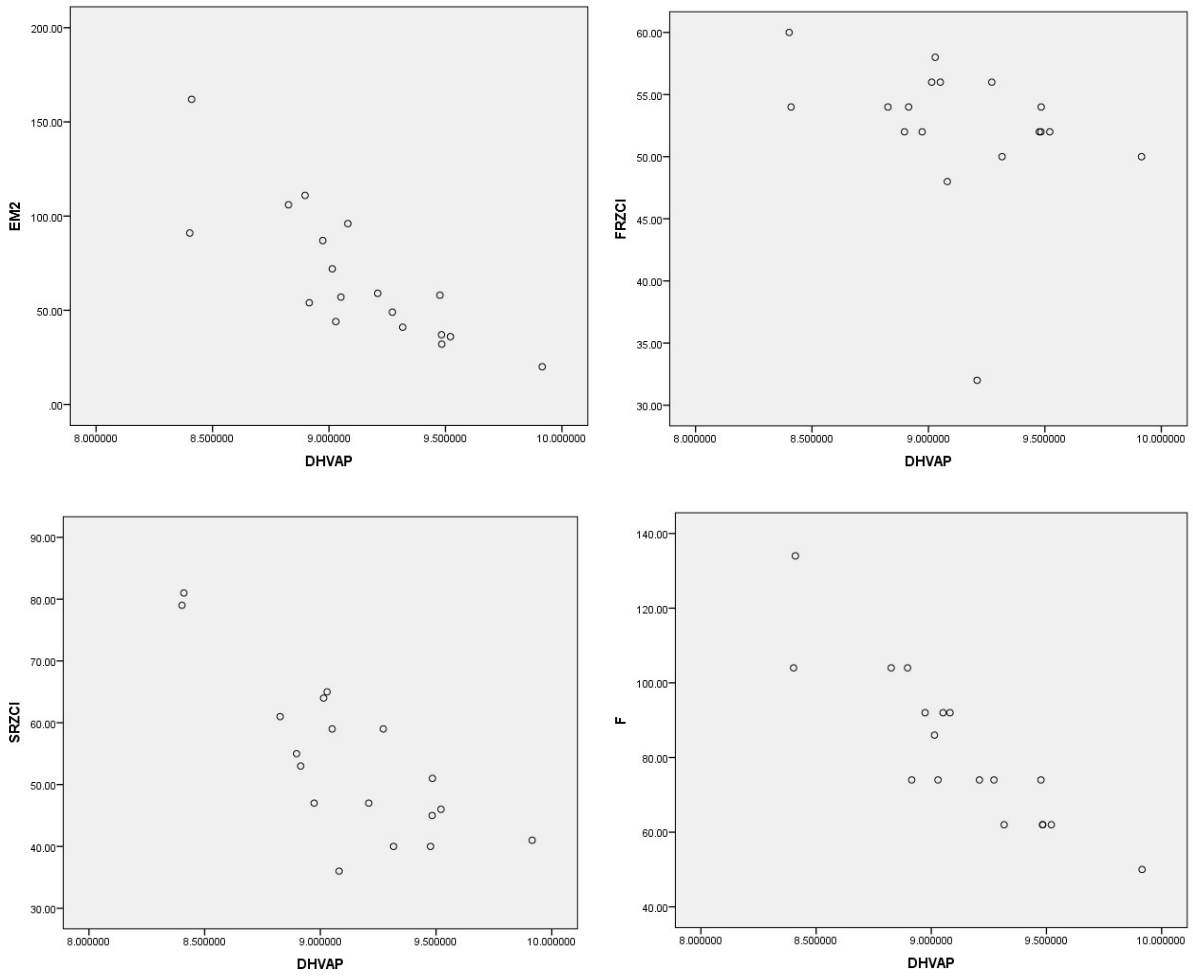
$$P = a + b\overline{EM_2}(G) \tag{13}$$

The correlation coefficients of physicochemical properties with individual M_1^a values show some significant results. The first mean Zagreb index is found to be useful to predict the DHVAP of octane isomers with correlation coefficient value 0.849 which is prediction power is better than second Zagreb index (0.801), second Zagreb coindex (0.819), reformulated Zagreb index (0.820), first reformulated Zagreb coindex (0.306) and second reformulated Zagreb coindex (0.780) respectively. Further, the predicting power of M_1^a in sensing acentric factor of octane isomers with correlation coeffiecnt value 0.831 is far better than the predicting power of other topological indices, such as first reformulated Zagreb coindex (0.063) and second reformulated Zagreb coindex (0.579) respectively. The one more application of M_1^a is to QSPR studies is found to be the prediction of entropy value of octane isomers with correlation coefficient value 0.810 which is far better than the first reformulated Zagreb coindex (0.138) and second reformulated Zagreb coindex (0.580) respectively.

The regression analysis of models (4)-(13) with single descriptors, reveals some interesting results for physicochemical properties of octane isomers. The range of R, S and F for each physical property of octane isomers are as follows:

For boiling point the range of R, S and F are 0.518 – 0.727, 0.351–4.574 and 7.131–20.996 respectively. Next, for critical temperature of octane isomers the range of R, S and F are 0.164 – 0.730, 6.8665 – 9.9589 and 0.262 –18.203 respectively, for critical pressure, density, heats of vaporization and heats formation all these parameters shows bad results. Finally for entropy and acentric factor of octane isomers above models (4-13) are most suitable models. As an example, we show the correlation coefficient of the above mentioned topological indices with the DHVAP of octane isomers in the following graphs:





Conclusion. The results of QSPR studies reveals that the regression model (3) is the most significant model to predict the physicochemical properties of molecular graphs. Hence the first mean Zagreb index is an important tool in the area of QSPR studies. Analogous to the second Zagreb index and forgotten index, we have defined the Second mean Zagreb index and forgotten mean index and results on the topics are under process.

References

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

[2] A. R. Ashrafi, T. Došlić, A. Hamzeh, Extremal graphs with respect to the Zagreb coindices, MATCH Commun. Math. Comput.Chem. 65 (2011) 85–92.

[3] J. Devillers, A. T. Balban, Topological indices and related descriptors in QSAR and QSPR, Gordon and Breach Science Publishers, Amsterdam, Netherlands, (1999).

[4] B. Furtula, I. Gutman(2015), A forgotten topological index. DOI 10.1007/s10910-015-0480-z

[5] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972), 535–538.

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

[7] I. Gutman, B. Furtula,, C. Elphick, Three new/old vertex-degree based topological indices, MATCH Commun. Math. Comput. Chem. 72(2014) 616–632.

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

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

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

[11] 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.

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

[13] A. Ilić, B. Zhou, On reformulated Zagreb indices, Discrete Appl. Math. 160 (2012) 204–209.

[14] A. Ilić, D. Stevanović, On comparing Zagreb indices, MATCH Commun. Math. Comput. Chem. 62 (2009), 681–687.

[15] M. Kuanar, S. K. Kuanar, B. K. Mishra, I. Gutman, Correlation of line graph parameters with physicochemical properties of octane isomers, Indian Journal of Chemistry 38A (1999) 525–528.

[16] 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.

[17] N. Trinajstić, Chemical graph theory, CRC Press (1992).