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Journal of Molecular Structure 1223 (2021) 129210

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: www.elsevier.com/locate/molstr

On neighborhood Zagreb index of product graphs

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ARTICLE INFO

Article history:
Received 17 July 2020
Revised 17 August 2020
Accepted 4 September 2020
Available online 6 September 2020

Keywords:
Molecular graph
Molecular descriptor
Neighborhood Zagreb index
Cartesian product
Tensor product
Wreath product

ABSTRACT

The properties and activities of chemicals are strongly related to their molecular structures. Topological indices defined on these molecular structures are capable to predict those properties and activities. In this article, a new topological index named as neighborhood Zagreb index (M_N) is presented. Here the chemical importance of the M_N index is investigated and it is shown that the newly introduced index is useful in predicting physico-chemical properties with high accuracy compared to some well-established and often used indices. The isomer-discrimination ability of M_N is also examined. To demonstrate how the computational formula of the novel index for chemical compounds is simple and convenient, the chemical structures of favipiravir and hydroxychloroquine are used. In addition, some explicit results for this index of different product graphs such as Cartesian, tensor and wreath product are derived. Some of these results are applied to obtain the M_N index of some special structures.

1. Introduction

A molecular graph [12,32] is a connected graph where loops and parallel connections are not allowed and in which nodes and edges are supposed to be atoms and chemical bonds of compound respectively. Throughout this work, we use only molecular graphs. For the node and edge sets of a graph G, we consider the notations $V(G)$ and $E(G)$, respectively. The degree (valency) of a node u, written as $deg_G(u)$, is the total count of edges associated with u. The set of neighbors of a node u is written as $N_G(u)$. For molecular graph, $|N_G(u)| = deg_G(u)$.

In mathematical chemistry, molecular descriptors play a leading role specifically in the field of quantitative structure property relationship/quantitative structure activity relationship modeling. Amongst them, an outstanding area is preserved for the well-known topological indices or graph invariants. A real valued mapping considering graph as an argument is called a graph invariant if it gives the same value to isomorphic graphs. The order(total count of nodes) and size(total count of edges) of a graph are examples of two graph invariants. In mathematical chemistry, the graph invariants are named as topological indices. Some familiar topological indices are Wiener index, Randić index, connectivity indices, Zagreb indices etc. The idea of topological indices was initiated when the eminent chemist Harold Wiener found the first topological index, known as Wiener index [6], in 1947 for searching boiling points of alkanes. Amidst the topological indices invented on initial stage, the Zagreb indices are associated with the most popular molecular descriptors. It was firstly presented by Gutman and Trinajestić [14], where they investigated how the total energy of π-electron depends on the structure of molecules and it was recognized on [13]. The first (M_1) and second (M_2) Zagreb indices are as follows:

$$M_1(G) = \sum_{u \in V(G)} deg_G(u)^2, \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} deg_G(u) deg_G(v). \tag{2}$$

For more discussion regarding the Zagreb indices, see the articles [4,5,11,22]. In addition to the Zagreb indices, there are some other well-established and most used degree based topological indices such as forgotten topological index (F) [8,14], Randić index (R) [30], sum connectivity index (SCI) [35] and symmetric division degree index (SDD) [33] to model different structure-property/structure-activity relationships, which are defined as follows.

$$F(G) = \sum_{u \in V(G)} deg_G(u)^3, \tag{3}$$

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg_G(u) deg_G(v)}}, \tag{4}$$

$$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg_G(u) + deg_G(v)}}, \tag{5}$$

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https://doi.org/10.1016/j.molstruc.2020.129210
0022-2860/

$$SDD(G) = \sum_{uv \in E(G)} \left[\frac{deg_G(u)}{deg_G(v)} + \frac{deg_G(v)}{deg_G(u)} \right]. \quad (6)$$

Let the degree sum of all nodes connected to u in G be denoted by $\delta_G(u)$, i.e.

$$\delta_G(u) = \sum_{v \in N_G(u)} deg_G(v). \quad (7)$$

Following the construction of first Zagreb index as described in Eq. (1), we present here a novel index known as the neighborhood Zagreb index(M_N) which is defined below.

$$M_N(G) = \sum_{u \in V(G)} \delta_G(u)^2. \quad (8)$$

In mathematical chemistry, graph operations are very significant since certain graphs of chemical interest can be evaluated by various graph operations of different simple graphs. H.Yousefi Azari and co-authors [3] derived some exact formulae of PI index for Cartesian product of bipartite graphs. P. Paulraja and V.S. Agnes [28] evaluated some explicit expressions of the degree distance for the Cartesian and wreath products. De et al. [25] found explicit expressions of the *F*-index under several graph operations. For further illustration on this area, interested readers are suggested some articles [1,2,9,10,15,19,24,26,29]. We continue this progress for M_N index. The objective of this work is to determine the usefulness of the newly designed index defined in Eq. (8) and compute some exact results for the index under different product graphs. Also we intend to apply that results to some special graphs and nanomaterials.

2. Materials and methods

Our main outcomes are organized in two parts. In the first part, the chemical applicability of the newly designed index is investigated. We consider the benchmark data set of octane isomers for such testing and corresponding experimental values of physicochemical properties are collected from www.moleculardescriptors.eu/dataset/dataset.htm. Different topological indices of octanes are obtained using Dev-C++ software. All the properties are correlated with the index by MATLAB. After that a regression analysis for well correlated properties is performed using MATLAB and Excel data analysis tools. Linear fittings of the obtained models are plotted by MATLAB basic fitting tools. The degeneracy of the indices are checked using "unique" command in MATLAB. In the second part, some explicit expressions of the novel index for different product graphs are computed. We consider combinatorial computing, graph theoretic tools and mathematical induction to obtain the results. Different composite graphs are drawn using Latex tikzpicture environment.

3. Results and discussion

Laboratory testing of chemicals to understand their different properties is very expensive. To overcome this, lots of topological indices have been presented in the theoretical chemistry. To introduce a topological index, one should check two aspects: On the one hand, it should correlate well with at least one physicochemical properties for a benchmark data set, while on the other hand its formulation should be simple and give some theoretical insight. We split this section into two subsections. Firstly, we establish the applicability of M_N index for octane isomer. We study the following linear regression model

$$P = I(\pm 2E) + S(\pm 2E)T, \quad (9)$$

where *P, I, E, S,* and *T* are properties, intercept, standard error of coefficients, slope, and topological index respectively. The results

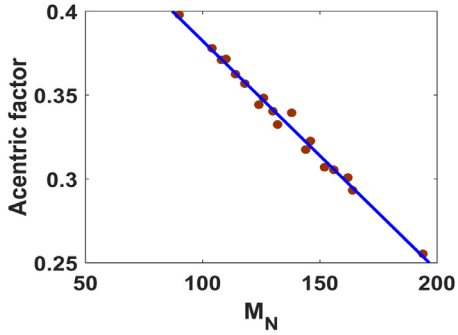


Fig. 1. Linear fitting of M_N with acentric factor for octane isomers.

are interpreted graphically using MATLAB software. Later, we study the index for some product graphs. Throughout this section, for the graph G_i, we use V_i and E_i for the node and the edge sets, respectively. Also for path, cycle and complete graphs with n nodes, we use P_n, C_n and K_n, respectively. From the definition (8), it is clear that $M_N(P_n) = 16n - 38$ $(n \geq 4)$, $M_N(C_n) = 16n$ $(n \geq 3)$, and $M_N(K_n) = n(n-1)^4$ $(n \geq 1)$. Since various significant graphs can be obtained from different product of P_n, C_n and K_n, the M_N index of them are also obtained in the second subsection.

3.1. Chemical significance of the neighborhood Zagreb index (M_N)

According to the instruction of the International Academy of Mathematical Chemistry (IAMC), to investigate the effectiveness of a topological index to model physico-chemical attributes, we use regression analysis. Usually octane isomers are helpful for such investigation, since they represent a sufficiently large and structurally diverse group of alkanes for the preliminary testing of indices [16,31]. Furtula et al. [8] derived that the correlation coefficient of both M_1 and *F* for octane isomers is greater than 0.95 with acentric factor and entropy. They also enhanced the skill of prediction of these indices by devising a linear model $(M_1 + \lambda F)$, where λ was varied from -20 to 20.

In this article, we find the correlation of entropy (S) and acentric factor with the neighborhood Zagreb index for octane isomers. The data related to octanes are listed in Table 1. Here we have computed that the correlation coefficient (r) between acentric factor and M_N is -0.99456 and between entropy (S) and M_N is -0.95261. Thus M_N can help to predict the entropy ($r^2 = 0.90746$) and acentric factor ($r^2 = 0.98915$) with powerful accuracy. These results confirm the suitability of the indices in QSPR analysis. The Eq. (9) yields the following regression models for the M_N index.

$$Acentric\,factor = 0.51918(\pm 0.00977) - 0.00137(\pm 7.16964 \times 10^{-5})M_N,$$
$$r^2 = 0.98915,\ S_e = 0.00381,\ F = 1457.77859,\ SF = 3.8081 \times 10^{-17}, \quad (10)$$

$$S = 127.80036(\pm 3.63605) - 0.16707(\pm 0.02667)M_N,$$
$$r^2 = 0.90746,\ S_e = 1.41645,\ F = 156.92469,\ SF = 1.1012 \times 10^{-9}, \quad (11)$$

where S_e, *F* and *SF* are the statistical parameters: standard error of model, F-test and significance F, respectively. The linear fittings of the models are depicted in Figs. 1 and 2. In both the figures, the solid circles represent the data point (x, y), where x, y denote the M_N value and the physico-chemical property for octane isomers, respectively and the blue line represents the regression line. The Fig. 1 reveals the strength of structure property relationship between M_N and acentric factor and the Fig. 2 shows that between M_N and acentric factor. If we round the r^2 values to two digits,

Table 1
Experimental values of the acentric factor, entropy(S) and the corresponding values of different topological indices for octane isomers.

Octane isomers	Acentric factor	S	M_N	M_1	M_2	F	SCI	R	SDD
n-octane	0.397898	111.67	90	26	24	50	3.6547	3.9142	15
2-methyl heptane	0.377916	109.84	104	28	26	62	3.5246	3.7701	17.3333
3-methyl heptane	0.371002	111.26	108	28	27	62	3.5491	3.8081	16.6667
4-methyl heptane	0.371504	109.32	110	28	27	62	3.5491	3.8081	16.6667
3-ethyl hexane	0.362472	109.43	114	28	28	62	3.5737	3.8461	16
2,2-dimethyl hexane	0.339426	103.42	138	32	30	92	3.3272	3.5607	21.75
2,3-dimethyl hexane	0.348247	108.02	126	30	30	74	3.4328	3.6807	18.6667
2,4-dimethyl hexane	0.344223	106.98	124	30	29	74	3.419	3.6639	19
2,5-dimethyl hexane	0.35683	105.72	118	30	28	74	3.3944	3.6259	19.6667
3,3-dimethyl hexane	0.322596	104.74	146	32	32	92	3.3656	3.6213	20.5
3,4-dimethyl hexane	0.340345	106.59	130	30	31	74	3.4574	3.7187	18
2-methyl-3-ethyl pentane	0.332433	106.06	132	30	31	74	3.4574	3.7187	18
3-methyl-3-ethyl pentane	0.306899	101.48	152	32	34	92	3.404	3.682	19.25
2,2,3-trimethyl pentane	0.300816	101.31	162	34	35	104	3.2442	3.4814	22.8333
2,2,4-trimethyl pentane	0.30537	104.09	156	34	32	104	3.1971	3.4165	24.0833
2,3,3-trimethyl pentane	0.293177	102.06	164	34	36	104	3.258	3.504	22.25
2,3,4-trimethyl pentane	0.317422	102.39	144	32	33	86	3.3165	3.5535	20.6667
2,2,3,3-tetramethyl butane	0.255294	93.06	194	38	40	134	3.0368	3.25	27.5

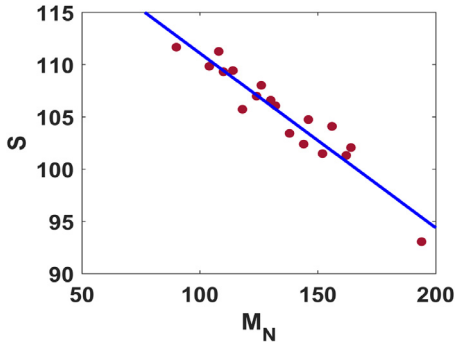


Fig. 2. Linear fitting of M_N with S for octane isomers.

Table 2
The square of correlation coefficient of different topological indices with acentric factor and entropy.

	M_1	M_2	F	SCI	R	SDD
Acentric factor	0.9468	0.973	0.9313	0.8647	0.8176	0.8118
S	0.9107	0.8868	0.9077	0.8518	0.8205	0.8276

then it is clear that 99% and 91% of our observations fit the models (10) and (11) respectively and are shown visually in Figs. 1 and 2 respectively. The data points in Fig. 1 are more closed to the best fitting line compared to the Fig. 2. It confirms that the linear fitting of the model (10) is more accurate that the model (11). The smaller the S_e values, the more confident we are regarding the regression equation. The S_e values of both the equations are significantly low. The average distance of the data points to the regression line is also very low in Figs. 1 and 2. In fact, Fig. 1 yields a lower average distance than Fig. 2. The consistency of the model improves as the F-value increases. In each model, F-value is considerably high. When the SF value is less than 0.05, then the model is considered to be statistically reliable. In each case, SF value is far less than 0.05. Correlation of some well-established and most used degree based indices like first (M_1) and second (M_2) Zagreb indices [14], forgotten topological index (F) [8,14], connectivity index (R) [30], sum connectivity index (SCI)[35] and symmetric division degree index (SDD) [33] with acentric factor and S is shown in Table 2. It reveals the supremacy of M_N compared to the indices in Table 2 in modelling acentric factor. Sometimes the novel index shows better predictive capability than the existing indices for S.

Table 3
Sensitivity of different indices for octane isomers.

Indices	Sensitivity (S_T)
M_1	0.333
M_2	0.722
F	0.389
R	0.889
SCI	0.889
SDD	0.889
Neighborhood Zagreb index (M_N)	**1.000**

Table 4
The square of correlation coefficient of M_N with some existing indices.

	M_1	M_2	F	SCI	R	SDD
M_N	0.9716	0.9646	0.9657	0.891	0.8471	0.8539

In addition to their application to different structure-property and structure-activity correlations, topological indices are also used for discrimination against isomers. The discrimination ability of an index has remarkable importance for the coding and the computer processing of chemical structures. Most of the indices have a flaw that more than one isomers occupy the same index which is known as degeneracy. But this novel index is exceptional for octane isomers. Konstantinova [21] proposed the sensitivity, the measure of degeneracy, formulated as

$$S_T = \frac{N - N_T}{N}, \tag{12}$$

where N and N_T are the total number of isomers and the count of isomers that cannot be discriminated by the descriptor T, respectively. The isomer discrimination ability of an index is directly proportional to S_T. Clearly, its maximum value is 1. Therefore, S_T plays a major role in the discriminating power of an index. The indices having good discrimination ability captures more structural information. For octane isomers, M_N index exhibits better response ($S_T = 1$) compared to some well established and most utilized degree based indices that are reported in Table 3.

Correlation of M_N with some existing indices are shown in Table 4.

Apart from chemical importance, an effective topological index should have a convenient and straightforward computational formula. To show how the computation of M_N index for chemical compound is clear and easy, we consider chemical structures favipiravir and hydroxychloroquine in Fig. 3. Favipiravir has been

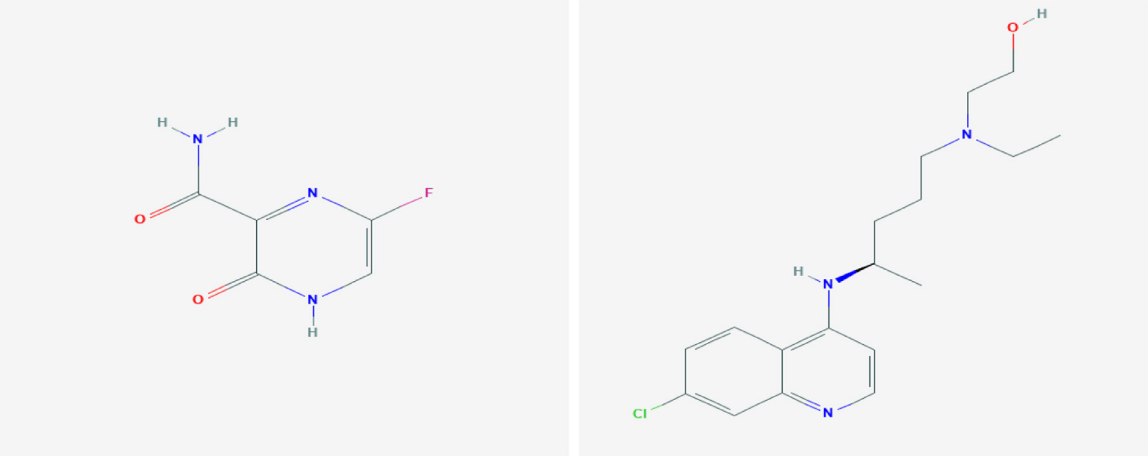


Fig. 3. Chemical structures of favipiravir and hydroxychloroquine from left to right.

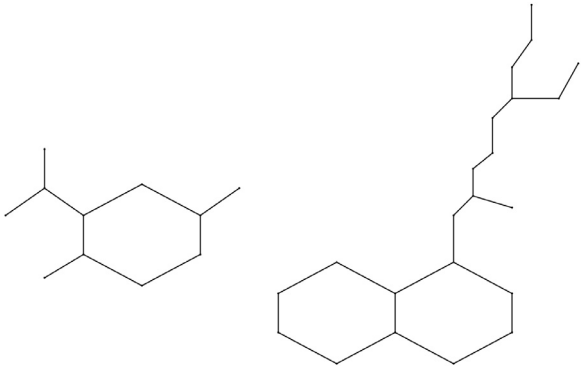


Fig. 4. Hydrogen deleted molecular graphs of favipiravir and hydroxychloroquine from left to right.

researched for the treatment of life-threatening pathogens such as Ebola, Lassa, and now COVID-19. Hydroxychloroquine is an antimalarial drug. It is one of the antiviral agents that is being investigated currently to prevent COVID-19. The hydrogen suppressed molecular graphs of the aforesaid compounds are shown in Fig. 4. Let G_1 and G_2 be the hydrogen deleted molecular graphs of favipiravir and hydroxychloroquine, respectively. Then, we have

$$M_N(G_1) = \sum_{u\in V(G_1)} \delta_G(u)^2 = 4(3)^2 + 4(5)^2 + 2(6)^2 + (8)^2 = 272,$$

$$M_N(G_2) = \sum_{u\in V(G_2)} \delta_G(u)^2 = 2(2)^2 + 2(3)^2 + 5(4)^2 + 8(5)^2 + 2(6)^2 + 2(7)^2 + (8)^2 = 540,$$

3.2. M_N Index of some product graphs

Product graphs are applicable in a number of areas, including automata theory, communication networks, information theory, computer architecture, algebraic structures and chemistry. They help to construct many network topologies for interconnection networks. In this section, we evaluate the newly introduced index for different product graphs such as Cartesian, wreath and tensor product of graphs. We proceed with the following lemma directly followed from definitions.

Lemma 3.1. *If G be a graph, then we have*

(i) $\sum_{u\in V(G)} \delta_G(u) = M_1(G)$,

(ii) $\sum_{u\in V(G)} deg_G(u)\delta_G(u) = 2M_2(G)$,

where $M_1(G)$, $M_2(G)$ are formulated in Eqs. (1), (2) and $\delta_G(u)$ is defined in Eq. (7).

3.2.1. Cartesian product

Definition 3.2. The Cartesian product of G_1, G_2, written as $G_1 \otimes G_2$, containing node set $V_1 \times V_2$ and (u_1, v_1) is connected to (u_2, v_2) iff [u_1 is connected with u_2 in G_1 and $v_1 = v_2$] or [v_1 is connected with v_2 in G_2 and $u_1 = u_2$]. We consider the symbol $\times$ for the Cartesian product of two sets.

Clearly the above definition yield the lemma stated below.

Lemma 3.3. *For graphs G_1 and G_2, we have*

(i) $\delta_{G_1\otimes G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v) + 2deg_{G_1}(u)deg_{G_2}(v)$,
(ii) $|E(G_1 \otimes G_2)| = |V_2||E_1| + |V_1||E_2|$.

In [18,20] different topological descriptors were studied for Cartesian product. Here we intend to go forward for the M_N index.

Proposition 3.4. *The M_N index of Cartesian product of G_1 and G_2 is given by*

$$M_N(G_1 \bigotimes G_2) = 6M_1(G_1)M_1G_2) + |V_2|M_N(G_1) + |V_1|M_N(G_2) + 16[|E_2|M_2(G_1) + |E_1|M_2(G_2)]. \quad (13)$$

Proof. From definition of neighborhood Zagreb index and applying Lemma 3.3 and Lemma 3.1, we get

$$\begin{aligned} M_N(G_1 \bigotimes G_2) &= \sum_{(u_1,u_2)\in V_1\times V_2} \delta^2_{G_1\otimes G_2}(u_1, u_2) \\ &= \sum_{u_1\in V_1}\sum_{u_2\in V_2} [\delta_{G_1}(u_1) + \delta_{G_2}(u_2) + 2deg_{G_1}(u_1)deg_{G_2}(u_2)]^2 \\ &= 6M_1(G_1)M_1G_2) + |V_2|M_N(G_1) + |V_1|M_N(G_2) + 16[|E_2|M_2(G_1) \\ &\quad +|E_1|M_2(G_2)]. \end{aligned}$$

Hence the result. Using the Eq. (13), we have the following results. □

Example 3.5. The Cartesian product of P_2 and P_{n+1} produces the ladder graph L_n (Fig. 5). By the above proposition, we derive the following result.

$$M_N(L_n) = 162n - 130, \ n \geq 3. \quad (14)$$

Carbon nanotube is the most popular nanomaterial having low weight, high strength, and very well thermal and electric conductivity. It has diverse usage in electromagnetic devices, Coatings and films, water and air filtration, bio-medical industry etc.

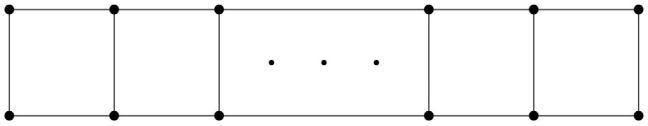


Fig. 5. The ladder graph L_n.

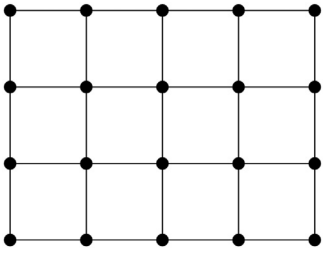


Fig. 6. The grid graph $P_5 \otimes P_4$.

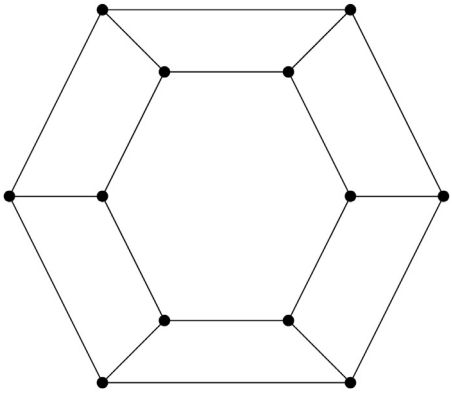


Fig. 7. The example of n-Prism graph ($n = 6$).

The M_N index for $C_4 - nanotorus$ and $C_4 - nanotube$ are obtained in Eqs. (15) and (16), respectively.

Example 3.6. For a $C_4 - nanotorus$ $TC_4(m, n) = C_m \otimes C_n$, the M_N index is given by

$$M_N(TC_4(m, n)) = 256mn. \tag{15}$$

Example 3.7. The Cartesian product of P_m and C_n yields a $C_4 - nanotube$ $TUC_4(m, n) = P_m \otimes C_n$. Its M_N index is as follows:

$$M_N(TUC_4(m, n)) = 256mn - 374n, \quad m \geq 4. \tag{16}$$

Example 3.8. The M_N index of the grid $(P_n \otimes P_m)$ (Fig. 6) is given by

$$M_N(P_n \bigotimes P_m) = 256mn - 374m - 374n + 472, \quad m, n \geq 4. \tag{17}$$

Example 3.9. For a n-prism $(K_2 \otimes C_n)$ (Fig. 7), the neighborhood Zagreb index is given below.

$$M_N(K_2 \bigotimes C_n) = 162n. \tag{18}$$

Example 3.10. The Cartesian product of K_n and K_m yields the rook's graph (Fig. 8). All legal move of a rook on a chessboard can be represented by a rook's graph. Its each node correspond to a square of the chessboard and edges correspond to legal moves from one square to another. Applying the Proposition 3.4, we have computed the M_N index of rook's graph as follows.

$$M_N(K_m \bigotimes K_n) = mn[2(m-1)(n-1)(2m^2 + 2n^2 + 3mn - 7m - 7n + 7) + (m-1)^4 + (n-1)^4]. \tag{19}$$

Now we generalize the Proposition 3.4. We begin with the following lemma.

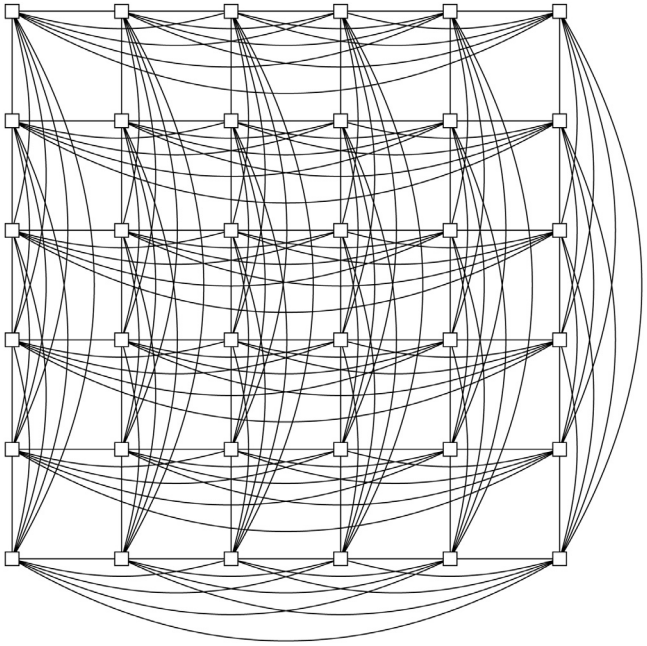


Fig. 8. The rook's graph $K_6 \otimes K_6$.

Lemma 3.11. *If G_1, G_2, ..., G_n be n graphs and $V = V(\bigotimes_{p=1}^{n} G_p)$, $E = E(\bigotimes_{p=1}^{n} G_p)$, then we have*

(i) $|E(\bigotimes_{p=1}^{n} G_p)| = |V| \sum_{p=1}^{n} \frac{|E_p|}{|V_p|}$,

(ii) $M_1(\bigotimes_{p=1}^{n} G_p) = |V| \sum_{p=1}^{n} \frac{M_1(G_p)}{|V_p|} + 4|V| \sum_{p\neq q, p,q=1}^{n-1} \frac{|E_p||E_q|}{|V_p||V_q|}$,

(iii) $M_2(\bigotimes_{p=1}^{n} G_p) = |V| \left[\sum_{p=1}^{n} \frac{M_2(G_p)}{|V_p|} + 4 \sum_{p\neq q\neq r, p,q,r=1}^{n} \frac{|E_p||E_q||E_r|}{|V_p||V_q||V_r|} \right] + 3 \sum_{p=1}^{n} M_1(G_p) \left(\frac{|E|}{|V_p|} - \frac{|V||E_p|}{|V_p|^2} \right)$.

Proof. Applying Lemma 3.3(ii) and an inductive argument, (i) is clear. In order to proof (ii) and (iii), we refer to Khalifeh et al. [19]. □

Proposition 3.12. *If G_1, G_2, ..., G_n be n graphs, then we have*

$$M_N(\bigotimes_{p=1}^{n} G_p) = |V| \left[\sum_{p=1}^{n} \frac{M_N(G_p)}{|V_p|} + 3 \sum_{p\neq q,\ p,q=1}^{n} \frac{M_1(G_p)M_1(G_q)}{|V_p||V_q|} + 24 \sum_{p\neq q\neq r,\ p,q,r=1}^{n} \frac{M_1(G_p)|E_q||E_r|}{|V_p||V_q||V_r|} + 16 \sum_{p\neq q,\ p,q=1}^{n} \frac{M_2(G_p)|E_q|}{|V_p||V_q|} + 16 \sum_{p\neq q\neq r\neq s,\ p,q,r,s=1}^{n} \frac{|E_p||E_q||E_r||E_s|}{|V_p||V_q||V_r||V_s|} \right]. \tag{20}$$

Proof. We derive the formula by mathematical induction. Evidently the result holds for $n = 2$. Let us take the proposition to be true for $(n-1)$ graphs. Then we obtain

$$M_N\left(\bigotimes_{p=1}^{n} G_p\right) = M_N\left(\bigotimes_{p=1}^{n-1} G_p \bigotimes G_n\right) = 6M_1\left(\bigotimes_{p=1}^{n-1} G_p\right) M_1(G_n) + |V_n| M_N\left(\bigotimes_{p=1}^{n-1} G_p\right) + |V\left(\bigotimes_{p=1}^{n-1} G_p\right)| M_N(G_n) + 16 \left[M_2\left(\bigotimes_{p=1}^{n-1} G_p\right) |E_n| + M_2(G_n) |E\left(\bigotimes_{p=1}^{n-1} G_p\right)| \right]. \tag{21}$$

Using Lemma 3.11 in Eq. (21), we get

$$\begin{aligned}M_N\left(\bigotimes_{p=1}^{n} G_p\right) &= 6|V|\frac{M_1(G_n)}{|V_n|}\left[\sum_{p=1}^{n-1}\frac{M_1(G_p)}{|V_p|}+4\sum_{p\neq q,\ p,q=1}^{n-1}\frac{|E_p||E_q|}{|V_p||V_q|}\right]\\ &+|V|\left[\sum_{p=1}^{n-1}\frac{M_N(G_p)}{|V_p|}+3\sum_{p\neq q,\ p,q=1}^{n-1}\frac{M_1(G_p)M_1(G_q)}{|V_p||V_q|}\right.\\ &+24\sum_{p\neq q\neq r,\ p,q,r=1}^{n-1}\frac{M_1(G_p)|E_q||E_r|}{|V_p||V_q||V_r|}+16\sum_{p\neq q,\ p,q=1}^{n-1}\frac{M_2(G_p)|E_q|}{|V_p||V_q|}\\ &\left.+16\sum_{p\neq q\neq r\neq s,\ p,q,r,s=1}^{n-1}\frac{|E_p||E_q||E_r||E_s|}{|V_p||V_q||V_r||V_s|}\right]+|V|\frac{M_N(G_n)}{|V_n|}\\ &+16\frac{|V|}{|V_n|}\left[|E_n|\{\sum_{p=1}^{n-1}\frac{M_2(G_p)}{|V_p|}+3\sum_{p=1}^{n-1}\frac{M_1(G_p)}{|V_p|}\left(\sum_{q=1}^{n-1}\frac{|E_q|}{|V_q|}-\frac{|E_p|}{|V_p|}\right)\right.\\ &\left.+4\sum_{p\neq q\neq r,\ p,q,r=1}^{n-1}\frac{|E_p||E_q||E_r|}{|V_p||V_q||V_r|}\}+M_2(G_n)\sum_{p=1}^{n-1}\frac{|E_p|}{|V_p|}\right].\end{aligned}$$

After simplification, we have

$$\begin{aligned}M_N\left(\bigotimes_{p=1}^{n} G_p\right) &= |V|\left[\sum_{p=1}^{n}\frac{M_N(G_p)}{|V_p|}+3\{\sum_{p\neq q,\ p,q=1}^{n-1}\frac{M_1(G_p)M_1(G_q)}{|V_p||V_q|}\right.\\ &+2\frac{M_1(G_n)}{|V_n|}\sum_{p=1}^{n-1}\frac{M_1(G_i)}{|V_p|}\}+24\{\sum_{p\neq q\neq r,\ p,q,r=1}^{n-1}\frac{M_1(G_p)|E_q||E_r|}{|V_p||V_q||V_r|}\\ &+\sum_{p\neq q,\ p,q=1}^{n-1}\frac{M_1(G_n)|E_p||E_q|}{|V_n||V_p||V_q|}+2\left(\sum_{p,q=1}^{n-1}\frac{M_1(G_p)|E_q||E_n|}{|V_p||V_q||V_n|}\right.\\ &\left.\left.-\sum_{p=1}^{n-1}\frac{M_1(G_p)|E_p||E_n|}{|V_p||V_p||V_n|}\right)\}+16\left\{\sum_{p\neq q,\ p,q=1}^{n-1}\frac{M_2(G_p)|E_q|}{|V_p||V_q|}\right.\right.\\ &\left.\left.+\sum_{p=1}^{n-1}\frac{M_2(G_n)|E_p|}{|V_n||V_p|}+\sum_{p=1}^{n-1}\frac{M_2(G_p)|E_n|}{|V_p||V_n|}\right\}\right]\\ &+16|V|\sum_{p\neq q\neq r\neq s,\ p,q,r,s=1}^{n}\frac{|E_p||E_q||E_r||E_s|}{|V_p||V_q||V_r||V_s|}.\end{aligned}\tag{22}$$

Thus, the result (20) can be obtained easily from the Eq. (22). □

Definition 3.13. Consider the graph G containing m-tuples $b_1, b_2, \ldots, b_m$ with $b_p \in \{0, 1, \ldots, n_p - 1\}$, $n_p \geqslant 2$, as vertices and let whenever the difference of two tuples is exactly one place, the corresponding two vertices are adjacent. This graph is known as Hamming graph. The necessary and sufficient criteria for a graph G to be a Hamming graph is that $G = \bigotimes_{p=1}^{m} K_{n_p}$ and that is why such a graph G is naturally written as $H_{n_1,n_2,\ldots,n_m}$.

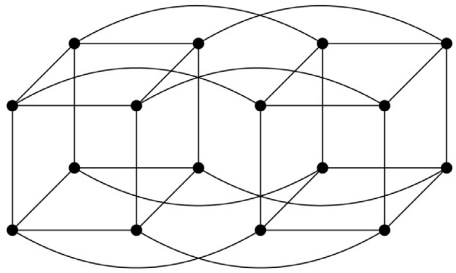
Hamming graph is very useful in coding theory specially in error correcting codes. Also such type of graph is effective in association schemes. Applying the result (20), we have the corollary stated below.

Corollary 3.14. *The neighborhood Zagreb index of Hamming graph is obtained as follows:*

$$\begin{aligned}M_N(G) = \prod_{p=1}^{m} n_p\left[\sum_{p=1}^{m}(n_p-1)^4+3\sum_{p\neq q,p,q=1}^{m}(n_p-1)^2(n_q-1)^2\right.\\ +6\sum_{p\neq q\neq r,p,q,r=1}^{m}(n_p-1)^2(n_q-1)(n_r-1)+4\sum_{p\neq q,p,q=1}^{m}(n_i-1)^3(n_j-1)\\ \left.+\sum_{p\neq q\neq r\neq s,p,q,r,s=1}^{m}(n_p-1)(n_q-1)(n_r-1)(n_s-1)\right].\end{aligned}$$

Example 3.15. When n_1, n_2, ...,n_m are all equal to 2, the graph $H_{n_1,n_2,\ldots,n_m}$ is known as a hyper cube (Fig. 9) with dimension m and written as Q_m. We compute the following.

$$M_N(Q_m) = 2^m m^4.\tag{23}$$



Q_4

Fig. 9. Example of Hypercube.

3.2.2. Tensor product

Definition 3.16. The tensor product of G_1, G_2, written as $G_1 \circledast G_2$, contains the node set $V_1 \times V_2$ and (u_1, v_1) is connected to (u_2, v_2) iff $u_1u_2 \in E_1$ and $v_1v_2 \in E_2$.

Clearly the definition gives the lemma as follows:

Lemma 3.17. *For graphs G_1 and G_2, we have*

$$\delta_{G_1 \circledast G_2}(u, v) = \delta_{G_1}(u)\delta_{G_2}(v).\tag{24}$$

The tensor product was thoroughly studied in terms of graph coloring, graph identification and decomposition, graph embedding, matching theory and graph stability in [17]. Z. Yarahmadi studied about degree based indices for tensor product in [34]. Also in [23,27] various topological descriptors of tensor product graphs are calculated. Here we continue this journey for the M_N index.

Proposition 3.18. *The M_N index of tensor product for G_1, G_2 is given by*

$$M_N(G_1 \circledast G_2) = M_N(G_1)M_N(G_2).\tag{25}$$

Proof. By the definition of the M_N index and applying Eq. (24), we get

$$\begin{aligned}M_N(G_1 \circledast G_2) &= \sum_{(u_1,u_2)\in V_1\times V_2}\delta^2_{G_1\circledast G_2}(u_1, u_2)\\ &= \sum_{u_1\in V_1}\sum_{u_2\in V_2}[\delta_{G_1}(u_1)\delta_{G_2}(u_2)]^2\\ &= M_N(G_1)M_N(G_2).\end{aligned}$$

Which is the required result. □

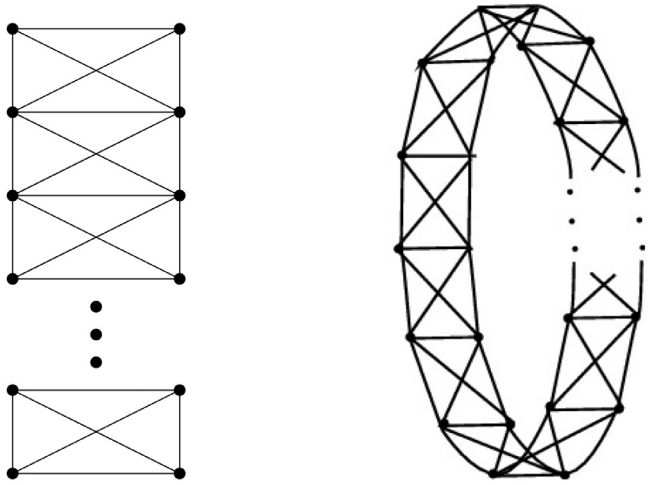
Example 3.19. Using the result (25), we have the following computations.

(i) $M_N(P_n \circledast P_m) = (16n - 38)(16m - 38)$, $m, n \geq 4$,
(ii) $M_N(C_n \circledast C_m) = 256mn$,
(iii) $M_N(K_n \circledast K_m) = mn(m-1)^4(n-1)^4$,
(iv) $M_N(P_n \circledast C_m) = 16m(16n - 38)$, $n \geq 4$,
(v) $M_N(P_n \circledast K_m) = m(m-1)^4(16n - 38)$, $n \geq 4$,
(vi) $M_N(C_n \circledast K_m) = 16mn(m-1)^4$.

3.2.3. Wreath product

Definition 3.20. The wreath product (also known as composition) of G_1 and G_2 having V_1 and V_2 as vertex sets with no common vertex and edge sets E_1 and E_2 is the graph $G_1[G_2]$ containing node set $V_1 \times V_2$ and (u_1, v_1) is connected to (u_2, v_2) iff $(u_1u_2 \in E_1)$ or $(u_1 = u_2$ and $v_1v_2 \in E_2)$.

From the definition, we have the following obvious lemma.



$P_n[P_2]$ $C_n[P_2]$

Fig. 10. Fence graph ($P_n[P_2]$) and closed fence graph ($C_n[P_2]$).

Lemma 3.21. *For graphs G_1 and G_2, we have*

$$\delta_{G_1[G_2]}(u,v) = |V_2|^2\delta_{G_1}(u) + \delta_{G_2}(v) + 2|E_2|deg_{G_1}(u) + |V_2|deg_{G_1}(u)deg_{G_2}(v). \quad (26)$$

In [7,25] different topological indices for wreath product of graphs are derived. Here we proceed for the M_N index of wreath product.

Proposition 3.22. *The M_N index of wreath product for G_1, G_2 is obtained as follows:*

$$M_N(G_1[G_2]) = |V_2|^5M_N(G_1) + |V_1|M_N(G_2) + 12|V_2||E_2|^2M_1(G_1) + 8|E_1||E_2|M_1(G_2) + 16|V_2|^3|E_2|M_2(G_1) + 8|V_2||E_1|M_2(G_2) + 3|V_2|^2M_1(G_1)M_1(G_2). \quad (27)$$

Proof. From definition of neighborhood Zagreb index and using Eq. (26), we have

$$\begin{aligned} M_N(G_1[G_2]) &= \sum_{(u,v)\in V_1\times V_2}\delta^2_{G_1[G_2]}(u,v) \\ &= \sum_{u\in V_1}\sum_{v\in V_2}[|V_2|^2\delta_{G_1}(u) + \delta_{G_2}(v) + 2|E_2|deg_{G_1}(u) \\ &\quad +|V_2|deg_{G_1}(u)deg_{G_2}(v)]^2 \\ &= \sum_{u\in V_1}\sum_{v\in V_2}[|V_2|^4\delta_{G_1}(u)^2 + |V_2|^2deg_{G_1}(u)^2deg_{G_2}(v)^2 + 4|E_2|^2deg_{G_1}(u)^2 \\ &\quad +\delta_{G_2}(v)^2 + 2|V_2|^3\delta_{G_1}(u)deg_{G_1}(u)deg_{G_2}(v) \\ &\quad +4|V_2|^2|E_2|\delta_{G_1}(u)deg_{G_1}(u) + 2|V_2|^2\delta_{G_1}(u)\delta_{G_2}(v) \\ &\quad +4|V_2||E_2|deg_{G_1}(u)^2deg_{G_2}(v) + 2|V_2|\delta_{G_2}(v)deg_{G_1}(u)deg_{G_2}(v) \\ &\quad +4deg_{G_1}(u)|E_2|\delta_{G_2}(v)]. \end{aligned}$$

Applying Lemma 3.1, we have

$$M_N(G_1[G_2]) = |V_2|^5M_N(G_1) + |V_1|M_N(G_2) + 12|V_2||E_2|^2M_1(G_1) + 8|E_1||E_2|M_1(G_2) + 16|V_2|^3|E_2|M_2(G_1) + 8|V_2||E_1|M_2(G_2) + 3|V_2|^2M_1(G_1)M_1(G_2),$$

which is the desired result. □

Example 3.23. The wreath product of the path graphs P_n and P_2 yield the fence graph (Fig. 10), whereas the wreath product of the cycle C_n and the path P_2 gives the closed fence graph (Fig. 10). Thus from the result (27), we compute the followings.

(i) $M_N(P_n[P_2]) = 1250n - 2560, \quad n \geqslant 4,$
(ii) $M_N(C_n[P_2]) = 1250n, \quad n \geqslant 3.$

4. Conclusion

In this article, we introduced the M_N index, examined its chemical applicability, computed some exact formulae for M_N of some product graphs and applied the results to some special graphs. As a future work, we derive the results for some other graph operations and compute some bounds of this index. Also some exact expressions of it for different networks can also be derived. As the pharmacological activity of a compound depends on its physicochemical properties and the correlations of M_N index with some of these properties are attractive, there is nothing to be surprised that M_N index can be used in designing new drugs.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Sourav Mondal: Conceptualization, Writing - original draft, Software. **Nilanjan De:** Conceptualization, Investigation, Writing - review & editing. **Anita Pal:** Supervision, Visualization, Validation.

Acknowledgments

The first author is very obliged to the Department of Science and Technology (DST), Government of India for the Inspire Fellowship [IF170148].

Supplementary material

Supplementary material associated with this article can be found, in the online version, at 10.1016/j.molstruc.2020.129210

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