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The Eccentric Zagreb Indices for the Subdivision of Some Graphs and Their Applications

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Abstract: Subdivision is one of the most important aspects of graph theory as it enables us to calculate the properties of some complicated graphs using some of the easier graphs. To understand the different properties of chemicals, laboratory tests must be performed, and this is extremely expensive. To overcome this problem, many topological indices in theoretical chemistry have been introduced and defined. In this paper, we calculate the eccentric Zagreb indices for the subdivision graphs of some graphs. Also, these indices were examined in their predictability of the boiling point of the chemical compounds.

Keywords: Eccentric Zagreb indices, Subdivision of graphs, Eccentricity of a vertex, Boiling point, Chemical compounds

1 Introduction

Let $G=(V,E)$ be a finite simple connected graph consists of a set of objects $V(G)$ called vertices, and another set $E(G)$ whose elements are called edges. The set $N(v)$ of all neighbors of $v \in V(G)$ is called the open neighborhood of v. Thus $N(v)=\{u \in V(G) : uv \in E(G)\}$. The degree $d_G(u)$ of a vertex u in G is define as $d_G(u)=|N(v)|$. The distance $d_G(u,v)$ between two vertices in a graph G is the length of the shortest path joining them [1]. For a vertex $v \in V(G)$ its eccentricity $\varepsilon_G(v)$ defined as

$$\varepsilon_G(v) = max_{u \in V(G)} d_G(v,u)$$

. The diameter of G is

$$D(G) = max_{v \in V(G)} \varepsilon_G(v)$$

and the radius of G is

$$r(G) = min_{v \in V(G)} \varepsilon_G(v)$$

. Hence $r(G) \leq \varepsilon_G(u) \leq D(G)$, for every $u \in V(G)$. We use the characters $C_n, K_{c,d}, S_{r+1}, W_{r+1}, K_n$ for the cycle, compete bipartite, star, wheel, complete graph respectively. Chemical graph theory is one of the branches of mathematical chemistry, as it is important and necessary for a better understanding and explanation of the nature of the chemical structure. By IUPAC terminology, a topological index is a numerical value correlation of chemical structure with different physical and chemical properties. In an exact phrase, topological indices are numerical parameters of the graph, such that these parameters are the same for the graph which they are isomorphism. We refer to [2,3,4,5,6,7,8,9,10,11,15,16,17,18] for some characteristics related to topological indices of graphs and molecular graphs. The beginning of topological indices was when chemist Wiener 1947 found the first topological index, known as the Winner index [12], to search for boiling points of chemical component and defined as

$$W(G) = \frac{1}{2} \sum_{\{u,v\} \in V(G)} d_G(u,v).$$

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Vukičević et al. [13] and Ghorbani et al. [14] introduced eccentricity Zagreb indices which are defined as:

$$M_1^*(G) = \sum_{uv \in E(G)} (\varepsilon_G(u) + \varepsilon_G(v)),$$

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

$$M_1^{**}(G) = \sum_{v \in V(G)} \varepsilon_G^2(v).$$

In this research work, we calculate the eccentric Zagreb indices for the subdivision of some graphs, and these indices were examined in their predictability of the boiling point of the chemical compounds. Also, we compare the correlation coefficient of eccentric Zagreb indices with a correlation coefficient of the Wiener index which is considered as the first index used to predict the boiling point of the chemical compound.

2 Eccentric Zagreb Indices for the Subdivision of Some Graphs

Subdivision is one of the most important aspects of graph theory as it enables us to calculate the properties of some complicated graphs using some of the easier graphs. Topological indices have become popular due to their application in chemistry in studying some chemical and physical properties of compounds or in related fields. In this section, we calculate eccentric Zagreb indices for the subdivision of some graphs.

Theorem 1.*For any cycle graph C_n, $n \geq 3$ vertices*

$$M_1^*(S(C_n)) = 4n^2,\ M_2^*(S(C_n)) = M_1^{**}(S(C_n)) = 2n^3.$$

*Proof.*Let C_n be a cycle, with $n \geq 3$ vertices.
Then $S(C_n) = C_{2n}$. So, the subdivision of C_n has $2n$ vertices. Thus, for any $v \in V(S(C_n))$ we get, $\varepsilon_{S(C_n)}(v) = n$. Hence,

$$M_1^*(S(C_n)) = 4n^2,\ M_2^*(S(C_n)) = M_1^{**}(S(C_n)) = 2n^3.$$

Theorem 2.*Let $S(S_{r+1})$ be the subdivision of star graph S_{r+1}, $r \geq 3$ vertices. Then*

$$M_1^*(S(S_{r+1})) = 12r,\ M_2^*(S(S_{r+1})) = 18r,$$

$$M_1^{**}(S(S_{r+1})) = 25r + 4.$$

*Proof.*Let $S(S_{r+1})$ be the subdivision of star graph S_{r+1}, $r \geq 3$ vertices. For any $v \in V(S(S_{r+1}))$ we have,

$$\varepsilon_{S(S_{r+1})}(v) = \begin{cases} 2, \text{ if } u \text{ is the center vertex;} \\ 3, \text{ if } d_{S_{r+1}}(v) = 2; \\ 4, \text{ if } u \text{ is pendent vertex.} \end{cases}$$

Hence, by using the definition of eccentric Zagreb indices we get the required.

Theorem 3.*Let $S(K_{c,d})$ be the subdivision of compete bipartite graph $K_{c,d}$, $c, d \geq 2$. Then*

$$M_1^*(S(K_{c,d})) = 16cd,\ M_2^*(S(K_{c,d})) = 32cd,$$

$$M_1^{**}(S(K_{c,d})) = 16(cd + c + d).$$

*Proof.*Let $S(K_{c,d})$ be the subdivision of compete bipartite graph $K_{c,d}$, $c, d \geq 2$. Note that, $D(S(K_{c,d})) = r(S(K_{c,d})) = \varepsilon_{S(K_{c,d})}(v) = 4$. Hence, $S(K_{c,d})$ is self-centered graph and by using the definition of eccentric Zagreb indices we get the following:

$$M_1^*(S(K_{c,d})) = 16cd,\ M_2^*(S(K_{c,d})) = 32cd,$$

$$M_1^{**}(S(K_{c,d})) = 16(cd + c + d).$$

Theorem 4.*For the complete graph K_n, $n \geq 4$ vertices*

$$M_1^*(S(K_n)) = 7n(n-1),\ M_2^*(S(K_n)) = 12n(n-1),$$

$$M_1^{**}(S(K_n)) = n(8n+1).$$

*Proof.*Let K_n be complete graph with $n \geq 4$ vertices. Let A be the set of all original vertices, and B be the set of entering vertices of $S(K_n)$. Hence,

$$\varepsilon_{S(K_n)}(v) = \begin{cases} 3, \text{ if } u \in A; \\ 4, \text{ if } u \in B. \end{cases}$$

And,

$$M_1^*(S(K_n)) = 7n(n-1),\ M_2^*(S(K_n)) = 12n(n-1),$$

$$M_1^{**}(S(K_n)) = n(8n+1).$$

The wheel graph W_{n+1} with $n+1$ vertices is defined to be the join of K_1 and C_n, where K_1 is the complete graph with one vertex and C_n is the cycle graph.

Theorem 5.*For the wheel graph W_{n+1}, $n \geq 6$*

$$M_1^*(S(W_{n+1})) = 38n,\ M_2^*(S(W_{n+1})) = 92n,$$

$$M_2^*(S(W_{n+1})) = 77n + 9.$$

*Proof.*Let W_{n+1} be the wheel graph with $n \geq 6$. Let w be the center vertex, A be the set of original vertices on the cycle, and B be the set of entering vertices on the cycle of the graph $S(W_{n+1})$. Hence,

$$\varepsilon_{S(W_{n+1})}(v) = \begin{cases} 3, \text{ if } u = w; \\ 4, \text{ if } uw \in E(S(W_{n+1})); \\ 5, \text{ if } u \in A; \\ 6, \text{ if } u \in B. \end{cases}$$

And,

$$M_1^*(S(W_{n+1})) = 38n,\ M_2^*(S(W_{n+1})) = 92n,$$

$$M_2^*(S(W_{n+1})) = 77n + 9.$$

Table 1: Eccentric Zagreb indices with Wiener index of primary amines.

Compound	$M_1^*(G)$	$M_2^*(G)$	$M_1^{**}(G)$	$W(G)$
n-propylamine	14	16	26	10
2-aminopropane	9	6	13	9
2-amino-2-methylproprane	12	8	17	16
2-aminobutane	19	22	35	18
2-methylpropylamine	19	22	35	18
n-butylamine	24	36	54	20
2-amino-2-methylbutane	24	28	44	28
2-aminopentane	31	48	70	32
3-methylbutylamine	31	48	70	31
2-methylbutylamine	29	42	63	32
n-pentylamine	38	73	100	35
4-methylpentylamine	47	93	125	50
n-hexylamine	54	124	163	56
3-methylpentylamine	45	85	116	50
4-aminoheptane	61	136	179	75
2-aminoheptane	65	154	199	79
n-heptylamine	74	200	252	84
n-octylamine	96	296	364	120
n-nonylamine	122	425	510	165
2-aminoundecane	169	670	785	275
3-aminopentane	29	42	63	31

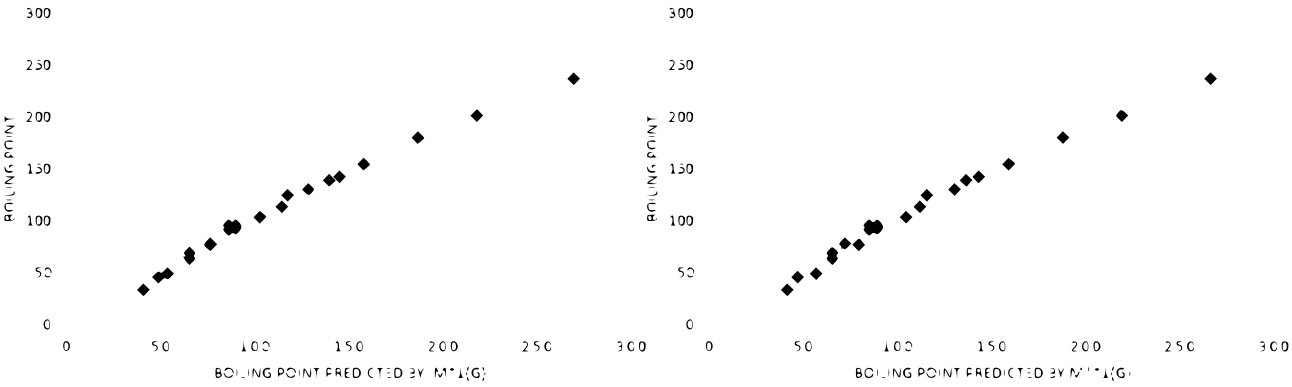

Fig. 1: Linear fitting of (a) $M_1^*(G)$ with pb (b) $M_1^{**}(G)$ with pb.

3 The Applications

To understand the different properties of chemicals, laboratory tests must be performed, and this is extremely expensive. To overcome this problem, many topological indices in theoretical chemistry have been introduced and defined. In this section, we define the significance of the eccentric Zagreb indices in determining the predicted boiling point of chemical compounds using nonlinear regression analysis. The primary amines group was adopted as a standard group in which the chemical and physical applicability of the eccentric Zagreb indices are tested. The value of boiling points is listed in Table 2. We calculate the Wiener index and eccentric Zagreb indices of primary amines and the data listed in Table 1. We get the relationship of eccentric Zagreb indices and Wiener index with boiling points of primary amines as in Table 2. In Table 3, we present correlation coefficient of boiling points predicted by eccentric Zagreb indices ($r = 0.9908$ to $r = 0.9935$) and Wiener index (0.9788) with boiling points of primary amines (see Fig 1,2). In Table 4, we determined the correlation coefficient of $M_1^*(G)$, $M_2^*(G)$ and $M_1^{**}(G)$ with $W(G)$. The nonlinear regression

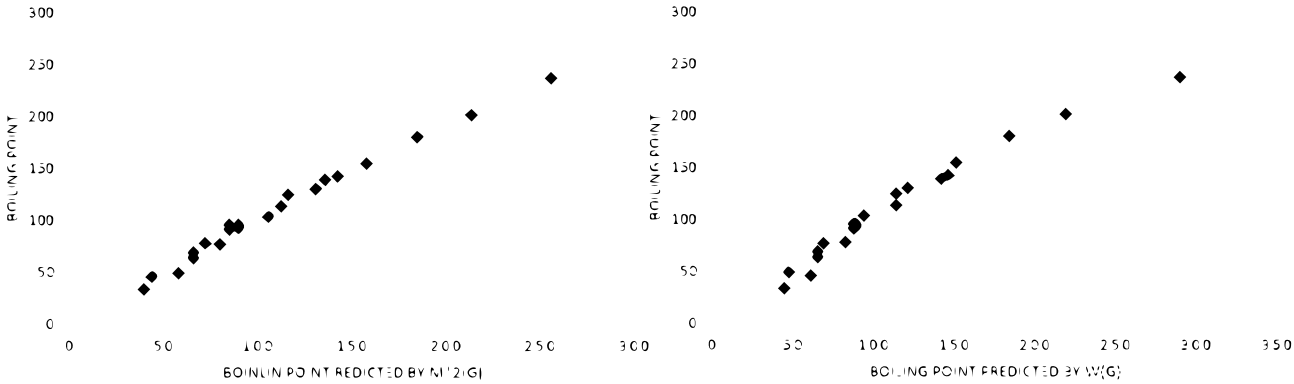

Fig. 2: Linear fitting of (a) $M_2^*(G)$ with pb (b) $W(G)$ with pb.

Table 2: Relationship of predicted boiling points calculated by eccentric Zagreb indices and Wiener index with boiling points of primary amines.

Compound	boiling point	bp$M_1^*(G)$	bp$M_2^*(G)$	bp $M_1^{**}(G)$	bp$W(G)$
n-propylamine	49	53.27	57.34	56.39	46.7
2-aminopropane	33	39.97	38.73	41.14	44.1
2-amino-2-methylproprane	46	48.19	43.46	46.48	60.52
2-aminobutane	63	64.97	65.13	46.57	64.57
2-methylpropylamine	69	46.97	65.13	64.57	64.57
n-butylamine	77	75.6	79.31	78.65	68.42
2-amino-2-methylbutane	78	75.62	71.73	71.65	82.33
2-aminopentane	92	89.31	88.99	88.51	88.6
3-methylbutylamine	96	89.31	88.99	88.51	87.07
2-methylbutylamine	96	85.52	84.36	84.36	88.6
n-pentylamine	104	101.94	105.23	104.1	93.08
4-methylpentylamine	125	117.05	115.94	115.2	113.25
n-hexylamine	130	128.1	130.08	130.01	120.54
3-methylpentylamine	114	113.79	111.84	111.37	113.25
4-aminoheptane	139	138.67	134.97	135.67	141.55
2-aminoheptane	142	144.5	141.85	142.37	145.65
n-heptylamine	155	157.22	157.49	158.5	150.65
n-octylamine	180	186.2	184.22	187.39	183.3
n-nonylamine	201	217.59	212.9	218.47	218.39
2-aminoundecane	237	268.93	255.42	265.84	289.23
3-aminopentane	91	85.52	84.36	84.36	87.07

analysis equations which are used are:

$$ln(bp) = 2.26 + 0.65\, ln(M_1^*(G)),$$

$$ln(bp) = 2.94 + 0.4\, ln(M_2^*(G)),$$

$$ln(bp) = 2.55 + 0.455\, ln(M_1^{**}(G)),$$

$$ln(bp) = 2.578 + 0.55\, ln(W(G)).$$

4 Conclusion

In this article, we have calculated eccentric Zagreb indices for some subdivisions of some graphs. These indices were examined in their predictability of the boiling point of the chemical compounds, as the correlation coefficients between 0.9908 and 0.9935 were obtained greater than those obtained in the case of the Wiener index.

Table 3: Correlation coefficient of boiling points predicted by eccentric Zagreb indices and Wiener index with boiling points of primary amines.

	bp predicted by $M_1^*(G)$	bp predicted by$M_2^*(G)$	bp predicted by$M_1^{**}(G)$	bp predicted by$W(G)$
bp	0.99199	0.9935	0.9908	0.9788

Table 4: Correlation coefficients of $M_1^*(G)$, $M_2^*(G)$ and $M_1^{**}(G)$ with $W(G)$.

	$M_1^*(G)$	$M_2^*(G)$	$M_1^{**}(G)$	$W(G)$
$M_1^*(G)$	1			
$M_2^*(G)$	0.9986	1		
$M_1^{**}(G)$	0.99938	0.9994	1	
$W(G)$	0.9939	0.9869	0.99068	1

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Conflicts of Interests

The authors declare that they have no conflicts of interests.

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