Available online at http://scik.org
J. Math. Comput. Sci. 10 (2020), No. 3, 639-655
https://doi.org/10.28919/jmcs/4396
ISSN: 1927-5307

# ZAGREB INDICES AT A DISTANCE 2

B. SOORYANARAYANA[1,*], S.B. CHANDRAKALA[2], G.R. ROSHINI[2]

[1]Department of Mathematics, Dr. Ambedkar Institute of Technology, Outer Ring Road, Bengaluru 560056, Karnataka State, India

[2]Department of Mathematics, Nitte Meenakshi Institute of Technology, Yelahanka 560064, Bengaluru, India



**Abstract.** In this paper, the first and the second Zagreb index at a distance $l$ which are denoted respectively as ${}_lM_1(G)$ and ${}_lM_2(G)$ are introduced and studied the special case when $l = 2$. Realization of ${}_2M_1(G)$ and ${}_2M_2(G)$ are studied along with some chemical applicability. The bounds of ${}_2M_1(G)$, ${}_2M_2(G)$, ${}_2M_1(\overline{G})$ and ${}_2M_2(\overline{G})$ are obtained for any $r$-regular graph $G$. Also, ${}_2M_1(G)$ and ${}_2M_2(G)$ are computed for cycloalkenes.

**Keywords:** topological indices; first Zagreb index; second Zagreb index; $r$-regular graph.

**2010 AMS Subject Classification:** 97K30, 05C07.

## 1. Introduction

Let $G$ be a simple, connected and undirected graph of order $O(G) = n$ and size $|E(G)| = m$. The degree of a vertex $v$ is the number of vertices adjacent to $v$ in $G$ and is denoted by $d_G(v)$. The distance between two vertices $u, v$ in $G$ is the length of a shortest path connecting $u$ and $v$ and is denoted by $d(u, v)$. Let $\overline{G}$ denote the compliment of a graph $G$. For undefined terminologies we refer to [2]. Also, similar work on degree based topological indices can be referred in [6, 7, 8].

*Corresponding author
E-mail address: dr_bsnrao@dr-ait.org
Received November 27, 2019

Topological index is a numerical value associated with a graph representing a molecule where atoms are represented as vertices and bonds as edges. One of the oldest topological indices is the well-known Zagreb indices which was in [1], first introduced by Gutman and Trinajstic and are defined as

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

and

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

The first Zagreb index and the second Zagreb index are defined over the edges of $G$. In 2016, Rizwana et al. [5] have introduced non-neighbor Zagreb indices, which are for the pair of distinct vertices $u, v$ with $d(u,v) \neq 1$. Analogous to this we define the generalized first and the second Zagreb indices of a graph $G$, namely the first Zagreb index and the second Zagreb index at a distance $l$, $1 \leq l \leq diam(G)$ respectively as :

$$_lM_1(G) = \sum_{d(u,v)=l} [d_G(u) + d_G(v)]$$

and

$$_lM_2(G) = \sum_{d(u,v)=l} d_G(u) d_G(v)$$

**Observation 1.1.** *For a complete graph $K_n$, the values $_2M_1(K_n)$ and $_2M_2(K_n)$ does not exist due to the fact that* $1 \leq l \leq diam(K_n) = 1$.

**Observation 1.2.** *Let $G$ be a connected graph of order atleast 3 which is not a clique. Then* $_2M_1(G) \geq 2$.

**Observation 1.3.** *Let $G$ be a connected graph of order atleast 3 which is not a clique. Then* $_2M_2(G) \geq 1$.

For the realization work of this paper we use the following theorems, which gives the necessary and sufficient condition for the existence of a graph $G$ of a given degree sequence, established during 1962 by Hakimi [3].

**Theorem 1.4** (Hakimi [3]). *The necessary and sufficient condition for positive integers $d_1 \leq d_2 \leq \cdots \leq d_n$ to be realizable (as the degrees of the vertices of a linear graph) are:*

*i)* $\sum_{i=1}^{n} d_i = 2e$, *e is an integer*

*ii)* $\sum_{i=1}^{n-1} d_i \geq d_n$.

**Theorem 1.5** (Hakimi [3]). *The necessary and sufficient condition for a set of integers* $d_1 \leq d_2 \leq \cdots \leq d_n$ *to be realizable as a connected graph are:*

*i) the set* $d_1, d_2, \ldots, d_n$ *is realizable.*

*ii)* $\sum_{i=1}^{n} d_i \geq 2(n-1)$.

In this paper, we consider the case of $l = 2$ in the newly defined Zagreb indices and compute ${}_2M_1(G)$ and ${}_2M_2(G)$ for some classes of graphs and cycloalkenes. We obtain the bounds of ${}_2M_1(G)$, ${}_2M_2(G)$, ${}_2M_1(\overline{G})$ and ${}_2M_2(\overline{G})$ for every $r$-regular graph $G$ with $O(G) = n$. Realization of ${}_2M_1(G)$ and ${}_2M_2(G)$ are studied and discussed their chemical applicability.

**Proposition 1.6.** *For a path* $P_n$ $(n \geq 4)$, ${}_2M_1(P_n) = 4n - 10$ *and* ${}_2M_2(P_n) = 4n - 12$.

**Proposition 1.7.** *For a cycle* $C_n$ $(n \geq 5)$, ${}_2M_1(C_n) = {}_2M_2(C_n) = 4n$.

**Proposition 1.8.** *For a star graph* $K_{1,n}$ $(n \geq 3)$, ${}_2M_1(K_{1,n}) = n(n-1)$ *and* ${}_2M_2(K_{1,n}) = \frac{n}{2}(n-1)$.

**Proposition 1.9.** *For a wheel graph* $W_{1,n}$ $(n \geq 4)$,

$$ {}_2M_1(W_{1,n}) = 3n(n-3) \text{ and } {}_2M_2(W_{1,n}) = \frac{9}{2}n(n-3). $$

## 2. Realization of ${}_2M_1(G)$

In this section, we give the existence of a graph of a given topological index namely ${}_2M_1(G)$.

**Lemma 2.1.** *For a connected graph G of order* $n \geq 3$, ${}_2M_1(G) \geq 2(n-2)$ *and the equality holds for* $G \cong K_n - e$.

*Proof.* To obtain minimal value for ${}_2M_1(G)$, we need a graph having the least number of pairs of vertices $(u,v)$ at a distance 2. This can be attained by removal of an edge from a complete graph $K_n$. Here only one pair of vertices is at distance 2. Further removal of edges from $K_n$ will increase the value of ${}_2M_1(G)$. Hence ${}_2M_1(G)$ is minimum for $G \cong K_n - e$. Also, ${}_2M_1(G) \geq 2(n-2)$. □

**Theorem 2.2.** *For any positive integer k, there is a connected graph G with* ${}_2M_1(G) = k$ *if and only if* $k \notin \{1,3,5,7,9,11,17\}$.

*Proof.* Let $G$ be a connected graph with ${}_2M_1(G) = k$. Suppose that $k \in \{1,3,5,7,9,11,17\}$. By Observation 1.2, ${}_2M_1(G) \geq 2$. Now we consider all possible graphs for different $O(G)$ and find ${}_2M_1(G)$. We observe that for $O(G) = 4 : {}_2M_1(G) \in \{4,6,8\}$, for $O(G) = 5 : {}_2M_1(G) \in \{6,10,12,13,14,15,16,18,20\}$ and for $O(G) = 6 : {}_2M_1(G) \in \{8, 14, 16, 18, 19, 20, 21, 22, 24, 25,26,27,28,29,30,32,34,36\}$. From Lemma 2.1 for $O(G) = 7 : {}_2M_1(G) \geq 10$ and $O(G) = 8 : {}_2M_1(G) \geq 12$. Hence there is no connected graph $G$ for ${}_2M_1(G) = \{1,3,5,7,9,11,17\}$.

Conversely, let $k$ be any positive integer and $k \notin \{1,3,5,7,9,11,17\}$. We prove the existence of $G$ in the following cases:

**Case 1:** $k \geq 32$ and $k \equiv 0 (mod\ 4)$.

Let $k = 4i$ for some integer $i \geq 8$. Consider the sequence $d_1, d_2, \ldots, d_i, d_{i+1}$, where $d_1 = d_2 = d_3 = d_4 = 1$, $d_j = 2$ for all $j, 5 \leq j \leq i-1$ and $d_i = d_{i+1} = 3$. Then $\sum_{j=1}^{i+1} d_j = 2(i) = 2(i+1-1)$ is even and $\sum_{j=1}^{i} d_j = 2(i-3)+3 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+1}$ as its degree sequence. One such graph is the graph $G$ of order $i+1$, obtained by $P_{i-1} : v_1 - v_2 - v_3 - \cdots - v_{i-1}$ by attaching two pendent vertices at $v_2$ and $v_{i-3}$, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 32 + \sum_{j=3}^{i-6} d_G(v_j) + d_G(v_{j+2}) = 4(i-8) + 32 = 4i = k$.

**Case 2:** $k \geq 21$ and $k \equiv 1 (mod\ 4)$.

Let $k = 21 + 4i$ for some integer $i \geq 0$. Consider the sequence $d_1, d_2, \ldots, d_i, d_{i+1}, \ldots, d_{i+6}$, where $d_1 = 1$, $d_j = 2$ for all $j, 2 \leq j \leq i+5$ and $d_{i+6} = 3$. Then $\sum_{j=1}^{i+6} d_j = 2(i+6) > 2(i+6-1)$ is even and $\sum_{j=1}^{i+5} d_j = 2(i+3)+3 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+6}$ as its degree sequence. One such graph is a tadpole graph $T_{4,i+2}$, of order $i+6$, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 25 + \sum_{j=1}^{i-1} d_G(v_j) + d_G(v_{j+2}) = 4(i-1) + 25 = 4i + 21 = k$.

**Case 3:** $k \equiv 2 (mod\ 4)$.

Let $k = 4i + 2$ for some integer $i \geq 0$. Consider the sequence $d_1, d_2, \ldots, d_i, d_{i+1}, d_{i+2}, d_{i+3}$, where $d_1 = d_2 = 1$ and $d_j = 2$ for all $j, 3 \leq j \leq i+3$. Then $\sum_{j=1}^{i+3} d_j = 2(i+2) = 2(i+3-1)$ is even and $\sum_{j=1}^{i+2} d_j = 2(i)+2 > 2 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+3}$ as its degree sequence. The path $P_{i+3}$ is one such graph for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 2(3) + \sum_{j=2}^{i} d_G(v_j) + d_G(v_{j+2}) = 4(i-1) + 2(3) = 4i + 2 = k$.

**Case 4:** $k \geq 19$ and $k \equiv 3(mod\ 4)$.

Let $k = 19 + 4i$ for some integer $i \geq 0$. Consider the sequence $d_1, d_2, \ldots, d_i, d_{i+1}, \ldots, d_{i+6}$, where $d_1 = 1$, $d_j = 2$ for all $j, 2 \leq j \leq i+3$ and $d_{i+4} = d_{i+5} = d_{i+6} = 3$. Then $\sum_{j=1}^{i+6} d_j = 2(i+7) > 2(i+6-1)$ is even and $\sum_{j=1}^{i+5} d_j = 2(i+4) + 3 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+6}$ as its degree sequence. One such graph is a graph $G$ obtained by identifying a vertex of degree 2 of $K_4 - e$ and one of the end vertices of $P_{i+3}$. For this graph $G$, ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 23 + \sum_{j=1}^{i-1} d_G(v_j) + d_G(v_{j+2}) = 4(i-1) + 23 = 4i + 19 = k$.

**Case 5:** $k = \{4, 8, 12, 13, 15, 16, 20, 24, 28\}$.

For $k = 4$. Consider the sequence $d_1, d_2, d_3, d_4$, where $d_1 = d_2 = 2$ and $d_3 = d_4 = 3$. Then $\sum_{j=1}^{4} d_j = 2(5) > 2(4-1)$ is even and $\sum_{j=1}^{3} d_j = 7 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4$ as its degree sequence. One such graph is a fan graph $F_{1,3}$, of order 4, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 1(2+2) = 4 = k$.

For $k = 8$. Consider the sequence $d_1, d_2, d_3, d_4$, where $d_1 = d_2 = d_3 = d_4 = 2$. Then $\sum_{j=1}^{4} d_j = 2(4) > 2(4-1)$ is even and $\sum_{j=1}^{3} d_j = 6 > 2 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4$ as its degree sequence. One such graph is a cycle $C_4$ for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 2(2+2) = 8 = k$.

For $k = 12$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = d_2 = d_3 = d_4 = 1$ and $d_5 = 4$. Then $\sum_{j=1}^{5} d_j = 2(4) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 4 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is a star graph $K_{1,4}$, of order 5, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 6(1+1) = 12 = k$.

For $k = 13$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = 1$, $d_2 = 2$ and $d_3 = d_4 = d_5 = 3$. Then $\sum_{j=1}^{5} d_j = 2(6) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 9 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence.

One such graph is a kite graph obtained by adding a new vertex to a vertex of degree 2 of $K_4 - e$ through an edge between them, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 2(1+3) + 1(2+3) = 13 = k$.

For $k = 15$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = 1$, $d_2 = d_3 = d_4 = 2$ and $d_5 = 3$. Then $\sum_{j=1}^{5} d_j = 2(5) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 7 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is $C_4$ with one pendent vertex, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 2(1+2) + 1(2+3) + 1(2+2) = 15 = k$.

For $k = 16$. Consider the sequence $d_1, d_2, d_3, d_4, d_5, d_6$, where $d_1 = d_2 = d_3 = 1$, $d_4 = d_5 = 2$ and $d_6 = 3$. Then $\sum_{j=1}^{6} d_j = 2(5) > 2(6-1)$ is even and $\sum_{j=1}^{5} d_j = 7 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5, d_6$ as its degree sequence. One such graph $G$ is a graph obtained by subdividing twice exactly one of the edges of $K_{1,3}$, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 1(1+1) + 3(1+2) + 1(2+3) = 16 = k$.

For $k = 20$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = d_2 = d_3 = d_4 = d_5 = 2$. Then $\sum_{j=1}^{5} d_j = 2(5) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 8 > 2 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is a cycle $C_5$ for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 5(2+2) = 20 = k$.

For $k = 24$. Consider the sequence $d_1, d_2, d_3, d_4, d_5, d_6$, where $d_1 = d_2 = d_3 = d_4 = d_5 = d_6 = 2$. Then $\sum_{j=1}^{6} d_j = 2(6) > 2(6-1)$ is even and $\sum_{j=1}^{5} d_j = 10 > 2 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5, d_6$ as its degree sequence. One such graph is a cycle $C_6$, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 6(2+2) = 24 = k$.

For $k = 28$. Consider the sequence $d_1, d_2, d_3, d_4, d_5, d_6, d_7, d_8$, where $d_1 = d_2 = d_3 = d_4 = 1$, $d_5 = d_6 = 2$ and $d_7 = d_8 = 3$. Then $\sum_{j=1}^{8} d_j = 2(7) = 2(8-1)$ is even and $\sum_{j=1}^{7} d_j = 11 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5, d_6, d_7, d_8$ as its degree sequence. One such graph $G$ is a graph obtained by two graphs $K_{1,3}$ and $P_4$ by adding an edge between one of the pendent vertices of $K_{1,3}$ and one of the non pendent vertex of $P_4$, for which ${}_2M_1(G) = \sum_{d(u,v)=2} d_G(u) + d_G(v) = 1(1+1)+4(1+2)+1(2+2)+1(3+3)+1(1+3) = 28 = k$.

Hence the theorem. □

## 3. REALIZATION OF ${}_2M_2(G)$

In this section, we give the existence of a graph of a given topological index namely ${}_2M_2(G)$.

**Lemma 3.1.** *For a connected graph $G$ of order $n \geq 3$, ${}_2M_2(G) \geq \frac{(n-1)(n-2)}{2}$ and the equality holds for $G \cong K_{1,n-1}$.*

*Proof.* To obtain minimal value for ${}_2M_2(G)$, we need a graph where degree of vertices are least for given pair of vertices $(u,v)$ whose $d(u,v) = 2$. This can be obtained for the graph $K_{1,n-1}$. If the degree of vertices are higher for pairs of vertices $(u,v)$ whose $d(u,v) = 2$, the value of ${}_2M_2(G)$ will increase. Hence ${}_2M_2(G)$ is minimum for $G \cong K_{1,n-1}$. Also, ${}_2M_2(G) \geq \frac{(n-1)(n-2)}{2}$. □

**Theorem 3.2.** *For any positive integer $k$, there is a connected graph $G$ with ${}_2M_2(G) = k$ if and only if $k \notin \{2,5,7\}$.*

*Proof.* Let $G$ be a connected graph with ${}_2M_2(G) = k$. Suppose that $k \in \{2,5,7\}$. Now we consider all possible graphs for different $O(G)$ and find ${}_2M_2(G)$. We observe that for $O(G) = 3 : {}_2M_2(G) \in \{1\}$, for $O(G) = 4 : {}_2M_2(G) \in \{3,4,8\}$, for $O(G) = 5 : {}_2M_2(G) \in \{6,8,9,10,11,12,14, 16,18,20,21\}$ and for $O(G) = 6 : {}_2M_2(G) \geq 10$ from Lemma 3.1. Hence there is no connected graph $G$ for ${}_2M_2(G) = \{2,5,7\}$.

Conversely, let $k$ be any positive integer and $k \notin \{2,5,7\}$. We prove the existence of $G$ in the following cases:

**Case 1:** $k \equiv 0(mod\ 4)$ .

Let $k = 4i$ for some integer $i \geq 1$. Consider the sequence $d_1, d_2, \ldots, d_i, d_{i+1}, d_{i+2}, d_{i+3}$, where $d_1 = d_2 = 1$ and $d_j = 2$ for all $j, 3 \leq j \leq i+3$. Then $\sum_{j=1}^{i+3} d_j = 2(i+2) = 2(i+3-1)$ is even and $\sum_{j=1}^{i+2} d_j = 2(i)+2 > 2 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+3}$ as its degree sequence. The path $P_{i+3}$ is one such graph for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 2(1\times 2) + \sum_{j=2}^{i} d_G(v_j)d_G(v_{j+2}) = 4(i-1)+4 = 4i = k$.

**Case 2:** $k \geq 13$ and $k \equiv 1(mod\ 4)$

Let $k = 13+4i$ for some integer $i \geq 0$. Consider the sequence $d_1, d_2, \ldots, d_i, d_{i+1}, \ldots, d_{i+6}$, where $d_1 = d_2 = d_3 = 1$, $d_j = 2$ for all $j, 4 \leq j \leq i+5$ and $d_{i+6} = 3$. Then $\sum_{j=1}^{i+6} d_j = 2(i+5) = 2(i+6-1)$ is even and $\sum_{j=1}^{i+5} d_j = 2(i+2)+3 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+6}$ as its degree sequence. One such graph is a graph $G$ of order $i+6$, obtained by $P_{i+5} : v_1 - v_2 - \cdots - v_{i+5}$ by attaching one pendent vertex at $v_2$, for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 13 + \sum_{j=3}^{i+2} d_G(v_j)d_G(v_{j+2}) = 4i+13 = k$.

**Case 3:** $k \geq 22$ and $k \equiv 2(mod\ 4)$.

Let $k = 22+4i$ for some integer $i \geq 0$. Consider the sequence $d_1, d_2, \ldots, d_i, \ldots, d_{i+8}$, where $d_1 = d_2 = d_3 = d_4 = 1$, $d_j = 2$ for all $j, 5 \leq j \leq i+6$ and $d_{i+7} = d_{i+8} = 3$. Then $\sum_{j=1}^{i+8} d_j = 2(i+7) = 2(i+8-1)$ is even and $\sum_{j=1}^{i+7} d_j = 2(i+4)+3 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+8}$ as its degree sequence. One such graph is a graph $G$ of order $i+8$, obtained by $P_{i+6} : v_1 - v_2 - \cdots - v_{i+6}$ by attaching two pendent vertices one at $v_2$ and other at $v_{i+5}$, for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 22 + \sum_{j=3}^{i+2} d_G(v_j)d_G(v_{j+2}) = 4i+22 = k$.

**Case 4:** $k \geq 19$ and $k \equiv 3(mod\ 4)$.

Let $k = 19+4i$ for some integer $i \geq 0$. Consider the sequence $d_1, d_2, \ldots, d_i, \ldots, d_{i+7}$, where $d_1 = d_2 = d_3 = 1$, $d_j = 2$ for all $j, 4 \leq j \leq i+6$ and $d_{i+7} = 3$. Then $\sum_{j=1}^{i+7} d_j = 2(i+6) = 2(i+7-1)$ is even and $\sum_{j=1}^{i+6} d_j = 2(i+3)+3 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+7}$ as its degree sequence. One such graph is a graph $G$ of order $i+7$, obtained by $P_{i+6} : v_1 - v_2 - \cdots - v_{i+6}$ by attaching one pendent vertex at $v_3$, for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 19 + \sum_{j=4}^{i+3} d_G(v_j)d_G(v_{j+2}) = 4i+19 = k$.

**Case 5:** $k = \{3, 6, 10, 11, 14, 15, 18\}$

For $k = 3$. Consider the sequence $d_1, d_2, d_3, d_4$, where $d_1 = d_2 = d_3 = 1$ and $d_4 = 3$. Then $\sum_{j=1}^{4} d_j = 2(3) = 2(4-1)$ is even and $\sum_{j=1}^{3} d_j = 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4$ as its degree sequence. One such graph is $K_{1,3}$ (star graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 3(1\times 1) = 3 = k$.

For $k = 6$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = d_2 = d_3 = d_4 = 1$ and $d_5 = 4$. Then $\sum_{j=1}^{5} d_j = 2(4) = 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 4 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is $K_{1,4}$ (star graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 6(1\times 1) = 6 = k$.

For $k = 10$. Consider the sequence $d_1, d_2, d_3, d_4, d_5, d_6$, where $d_1 = d_2 = d_3 = d_4 = d_5 = 1$ and $d_6 = 5$. Then $\sum_{j=1}^{6} d_j = 2(5) = 2(6-1)$ is even and $\sum_{j=1}^{5} d_j = 5 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5, d_6$ as its degree sequence. One such graph is $K_{1,5}$ (star graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 10(1\times 1) = 10 = k$.

For $k = 11$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = 1$, $d_2 = d_3 = d_4 = 2$ and $d_5 = 3$. Then $\sum_{j=1}^{5} d_j = 2(5) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 7 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is $T_{3,2}$ (tadpole graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 1(1\times 3) + 2(2\times 2) = 11 = k$.

For $k = 14$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = 1$, $d_2 = d_3 = d_4 = 2$ and $d_5 = 3$. Then $\sum_{j=1}^{5} d_j = 2(5) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 7 > 3 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is $T_{4,1}$ (tadpole graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 2(1\times 2) + 1(2\times 3) + 1(2\times 2) = 14 = k$.

For $k = 15$. Consider the sequence $d_1, d_2, d_3, d_4, d_5, d_6, d_7$, where $d_1 = d_2 = d_3 = d_4 = d_5 = d_6 = 1$ and $d_7 = 6$. Then $\sum_{j=1}^{7} d_j = 2(6) = 2(7-1)$ is even and $\sum_{j=1}^{6} d_j = 6 = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5, d_6, d_7$ as its degree sequence. One such graph is $K_{1,6}$ (star graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 15(1\times 1) = 15 = k$.

For $k = 18$. Consider the sequence $d_1, d_2, d_3, d_4, d_5$, where $d_1 = d_2 = d_3 = d_4 = 3$ and $d_5 = 4$. Then $\sum_{j=1}^{5} d_j = 2(8) > 2(5-1)$ is even and $\sum_{j=1}^{4} d_j = 12 > 4 = d_n$. So, by

Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, d_3, d_4, d_5$ as its degree sequence. One such graph is $W_{1,4}$ (wheel graph), for which ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 2(3\times 3) = 18 = k$.

Hence the theorem. □

**Proposition 3.3.** *For every perfect square k, there is a graph G with* ${}_2M_2(G) = k$. *Moreover, the graph* $G \cong K_{\sqrt{k}+2} - e$.

*Proof.* Let $k = i^2$ for some integer $i \geq 1$. Consider the sequence $d_1, d_2, \ldots, d_{i+2}$, where $d_1 = d_2 = i$ and $d_j = (i+1)$ for all $j, 3 \leq j \leq i+2$. Then $\sum_{j=1}^{i+2} d_j = 2i(\frac{i}{2} + \frac{3}{2}) > 2(i+2-1)$ is even and $\sum_{j=1}^{i+1} d_j = i(i+2) - 1 > (i+1) = d_n$. So, by Theorem 1.5, there is a connected graph $G$ with $d_1, d_2, \ldots, d_{i+2}$ as its degree sequence. But then $G \cong K_{\sqrt{k}+2} - e$ and hence ${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = 1(i\times i) = i^2 = k$ implies that $G$ is the required graph with ${}_2M_2(G) = k$ and is of order $(\sqrt{k}+2)$. □

## 4. Bounds for $r$-Regular Graph

We begin this section with the following theorems which gives the upper bound of ${}_2M_1(G)$ and ${}_2M_2(G)$ for any $r$-regular graph of $G$.

**Theorem 4.1.** *For any r-regular graph G of order* $n \geq 5$, ${}_2M_1(G) \leq nr^2(r-1)$.

*Proof.* For any $r$-regular graph $G$ of order $n \geq 5$, for each $u \in V(G)$ there are at most $r(r-1)$ vertices at a distance 2.

$${}_2M_1(G) = \sum_{d(u,v)=2} [d_G(u) + d_G(v)] = \sum_{d(u,v)=2} 2r \leq \frac{nr(r-1)(2r)}{2} \leq nr^2(r-1).$$

Equality holds for 2-regular graphs. □

**Theorem 4.2.** *For any r-regular graph G of order* $n \geq 5$, ${}_2M_2(G) \leq \frac{n}{2}r^3(r-1)$.

*Proof.* For any $r$-regular graph $G$ of order $n \geq 5$, for each $u \in V(G)$ there are at most $r(r-1)$ vertices at a distance 2.

$${}_2M_2(G) = \sum_{d(u,v)=2} d_G(u)d_G(v) = \sum_{d(u,v)=2} r^2 \leq \frac{nr(r-1)(r^2)}{2} \leq \frac{n}{2}r^3(r-1).$$

Equality holds for 2-regular graphs. □

We now obtain the sharp lower and the upper bound of ${}_2M_1(G)$, ${}_2M_2(G)$, ${}_2M_1(\overline{G})$ and ${}_2M_2(\overline{G})$ for a given $r$-regular graph $G$.

**Proposition 4.3.** *For a r-regular graph G of order n, if* $S = \{\{u,v\} \mid u,v \in V(G) \text{ and } d(u,v) = 2\}$ *then* $\mid S \mid$ *is maximum for* $diam(G) = 2$.

**Theorem 4.4.** *For a given r-regular graph G of order n;* $4n \leq {}_2M_1(G) \leq nr(n-1-r)$. *Further, the equality holds for* $n = 5, r = 2$.

*Proof.* For the lower bound: Graph $G \cong C_n$ is the only regular graph with the least value of ${}_2M_1(G)$. Therefore, ${}_2M_1(G) \geq {}_2M_1(C_n) = 4n$ by Proposition 1.7.

For the upper bound: Let $S = \{\{u,v\} \mid u,v \in V(G) \text{ and } d(u,v) = 2\}$. For regular graph $G$ of regularity $r$, ${}_2M_1(G) = 2r \mid S \mid$. By Proposition 4.3, we consider regular graph of $diam = 2$. Now, $\mid S \mid = \frac{n(n-1)}{2} - \frac{nr}{2} = \frac{n}{2}(n-1-r)$. ${}_2M_1(G) \leq nr(n-1-r)$.

Maximality of ${}_2M_1(G)$ is discussed in the following cases:

(i) When $n$ is even $(n \geq 8)$ for $r = \frac{n}{2}$ and $r = \frac{n}{2} - 1$, ${}_2M_1(G) = \frac{n^2}{4}(n-2)$.

(ii) When $n = 4k+1$ $(n \geq 5)$ for $r = \frac{(n-1)}{2}$, ${}_2M_1(G) = \frac{n}{4}(n-1)^2$.

(iii) When $n = 4k+3$ $(n \geq 11)$ for $r = \frac{(n+1)}{2}$ and $r = \frac{(n+1)}{2} - 2$, ${}_2M_1(G) = \frac{n}{4}(n+1)(n-3)$.

□

**Theorem 4.5.** *For a given r-regular graph G of order n;* $4n \leq {}_2M_2(G) \leq \frac{nr^2}{2}(n-1-r)$. *Further, the equality holds for* $n = 5, r = 2$.

*Proof.* For the lower bound: Graph $G \cong C_n$ is the only regular graph with the least value of ${}_2M_2(G)$. Therefore, ${}_2M_2(G) \geq {}_2M_2(C_n) = 4n$ by Proposition 1.7.

For the upper bound: Let $S = \{\{u,v\} \mid u,v \in V(G) \text{ and } d(u,v) = 2\}$. For regular graph $G$ of regularity $r$, ${}_2M_2(G) = r^2 \mid S \mid$. By Proposition 4.3, we consider regular graph of $diam = 2$. Now, $\mid S \mid = \frac{n(n-1)}{2} - \frac{nr}{2} = \frac{n}{2}(n-1-r)$. ${}_2M_2(G) \leq \frac{nr^2}{2}(n-1-r)$.

Maximality of ${}_2M_2(G)$ is discussed in the following cases:

(i) when $n = 6k$ $(k \geq 1)$ for $r = \frac{n}{2} + (k-1)$, ${}_2M_2(G) = \frac{n}{16}(n-2+2k)^2(n-2k)$.

(ii) when $n = 6k+1$ $(k \geq 1)$ for $r = \frac{\lceil n \rceil}{2} + (k-1)$, ${}_2M_2(G) = \frac{n}{16}(n-1+2k)^2(n-2k-1)$.

(iii) when $n = 6k+2$ $(k \geq 1)$ for $r = \frac{n}{2} + k$, ${}_2M_2(G) = \frac{n}{16}(n+2k)^2(n-2k-2)$.

(iv) when $n = 6k+3$ $(k \geq 1)$ for $r = \frac{\lceil n \rceil}{2} + k$, ${}_2M_2(G) = \frac{n}{16}(n+1+2k)^2(n-2k-3)$.

(v) when $n = 6k+4$ $(k \geq 1)$ for $r = \frac{n}{2} + k$, ${}_2M_2(G) = \frac{n}{16}(n+2k)^2(n-2k-2)$.

(vi) when $n = 6k+5$ $(k \geq 1)$ for $r = \frac{\lfloor n \rfloor}{2} + k$, ${}_2M_2(G) = \frac{n}{16}(n-1+2k)^2(n-2k-1)$.

□

**Theorem 4.6.** *For a given r-regular graph G of order n;* $4n \leq {}_2M_1(\overline{G}) \leq nr(n-1-r)$. *Further, the equality holds for* $n = 5, r = 2$.

*Proof.* For the lower bound: ${}_2M_1(\overline{G})$ is minimum when $G$ is of regularity $r = n-3 \Rightarrow \overline{G}$ is of regularity 2. Hence, $\overline{G} \cong C_n$. Therefore, ${}_2M_1(\overline{G}) \geq {}_2M_1(C_n) = 4n$ by Proposition 1.7.

For the Upper bound: Let $S = \{\{u,v\} \mid u,v \in V(\overline{G}) \textit{ and } d(u,v) = 2\}$. For regular graph $G$ of regularity $r$, ${}_2M_1(\overline{G}) = 2(n-1-r) \mid S \mid$. By Proposition 4.3, we consider regular graph of $diam = 2$. Now, $\mid S \mid = \frac{n(n-1)}{2} - \frac{n(n-1-r)}{2} = \frac{nr}{2}$. ${}_2M_1(\overline{G}) \leq nr(n-1-r)$.

Maximality of ${}_2M_1(\overline{G})$ is discussed in the following cases:

(i) When $n$ is even $(n \geq 8)$ for $r = \frac{n}{2}$ and $r = \frac{n}{2} - 1$, ${}_2M_1(\overline{G}) = \frac{n^2}{4}(n-2)$.

(ii) When $n = 4k+1$ $(n \geq 5)$ for $r = \frac{(n-1)}{2}$, ${}_2M_1(\overline{G}) = \frac{n}{4}(n-1)^2$.

(iii) When $n = 4k+3$ $(n \geq 11)$ for $r = \frac{(n+1)}{2}$ and $r = \frac{(n+1)}{2} - 2$, ${}_2M_1(\overline{G}) = \frac{n}{4}(n+1)(n-3)$.

□

**Theorem 4.7.** *For a given r-regular graph G of order n;* $4n \leq {}_2M_2(\overline{G}) \leq \frac{nr}{2}(n-1-r)^2$. *Further, the equality holds for* $n = 5, r = 2$.

*Proof.* For the lower bound: ${}_2M_2(\overline{G})$ is minimum when $G$ is of regularity $r = n-3 \Rightarrow \overline{G}$ is of regularity 2. Hence, $\overline{G} \cong C_n$. Therefore, ${}_2M_2(\overline{G}) \geq {}_2M_2(C_n) = 4n$ by Proposition 1.7.

For the upper bound: Let $S = \{\{u,v\} \mid u,v \in V(\overline{G}) \textit{ and } d(u,v) = 2\}$. For regular graph $G$ of regularity $r$, ${}_2M_2(\overline{G}) = (n-1-r)^2 \mid S \mid$. By Proposition 4.3, we consider regular graph of $diam = 2$. Now, $\mid S \mid = \frac{n(n-1)}{2} - \frac{n(n-1-r)}{2} = \frac{nr}{2}$. ${}_2M_2(\overline{G}) \leq \frac{nr}{2}(n-1-r)^2$.

Maximality of ${}_2M_2(\overline{G})$ for regular graph $\overline{G}$ of regularity $\overline{r}$, is discussed in the following cases:

(i) when $n = 6k$ $(k \geq 1)$ for $\overline{r} = \frac{n}{2} + (k-1)$, ${}_2M_2(\overline{G}) = \frac{n}{16}(n-2+2k)^2(n-2k)$.

(ii) when $n = 6k+1$ $(k \geq 1)$ for $\overline{r} = \frac{\lceil n \rceil}{2} + (k-1)$, ${}_2M_2(\overline{G}) = \frac{n}{16}(n-1+2k)^2(n-2k-1)$.

(iii) when $n = 6k+2$ $(k \geq 1)$ for $\overline{r} = \frac{n}{2} + k$, ${}_2M_2(\overline{G}) = \frac{n}{16}(n+2k)^2(n-2k-2)$.

(iv) when $n = 6k+3$ $(k \geq 1)$ for $\bar{r} = \frac{\lceil n \rceil}{2} + k$, ${}_2M_2(\overline{G}) = \frac{n}{16}(n+1+2k)^2(n-2k-3)$.

(v) when $n = 6k+4$ $(k \geq 1)$ for $\bar{r} = \frac{n}{2} + k$, ${}_2M_2(\overline{G}) = \frac{n}{16}(n+2k)^2(n-2k-2)$.

(vi) when $n = 6k+5$ $(k \geq 1)$ for $\bar{r} = \frac{\lfloor n \rfloor}{2} + k$, ${}_2M_2(\overline{G}) = \frac{n}{16}(n-1+2k)^2(n-2k-1)$.

□

## 5. ${}_2M_1(G)$ AND ${}_2M_2(G)$ OF CYCLOALKENES

In this section, we consider cycloalkene $C_n^{2n-2}$ having $n$ carbon atoms and $(2n-2)$ hydrogen atoms and alkyl $R_r, r \in \mathbb{Z}^+$ attached instead of hydrogen atom in cycloalkenes which is denoted as $C_n^{R_r}$ [4]. We obtain ${}_2M_1(G)$ and ${}_2M_2(G)$ for these cycloalkenes.

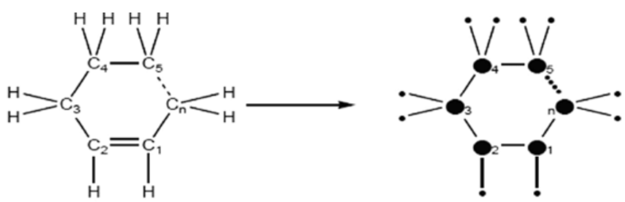


FIGURE 1. Cycloalkene and its graph model $C_n^{2n-2}$.

**Theorem 5.1.** *Let $n \geq 5$ be a positive integer. Then for a graph $C_n^{2n-2}$,*

$$ {}_2M_1(C_n^{2n-2}) = 2(15n-17) \text{ and } {}_2M_2(C_n^{2n-2}) = 33n-40. $$

*Proof.* Let $G = C_n^{2n-2}$ and $S = \{\{u,v\} \mid u,v \in V(G) \text{ and } d(u,v) = 2\}$. $\mid V(G) \mid = 3n-2$ and $\mid S \mid = 6n-6$. In $G$, there are two vertices of degree 3, $(n-2)$ vertices of degree 4 and $(2n-2)$ vertices of degree 1. Then,

$$
\begin{aligned}
{}_2M_1(C_n^{2n-2}) &= \sum_{d(u,v)=2} [d_G(u) + d_G(v)] \\
&= 4(4+3) + (n-4)(4+4) + 6(1+3) + (4n-10)(1+4) + (n-2)(1+1) \\
&= 2(15n-17)
\end{aligned}
$$

and

$$
\begin{aligned}
{}_2M_2(C_n^{2n-2}) &= \sum_{d(u,v)=2} d_G(u)d_G(v) \\
&= 4(4\times 3)+(n-4)(4\times 4)+6(1\times 3)+(4n-10)(1\times 4)+(n-2)(1\times 1) \\
&= 33n-40
\end{aligned}
$$

Hence the theorem. □

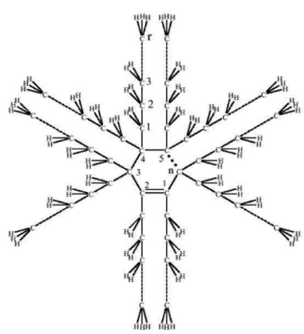

FIGURE 2. Structure of $C_n^{R_r}$

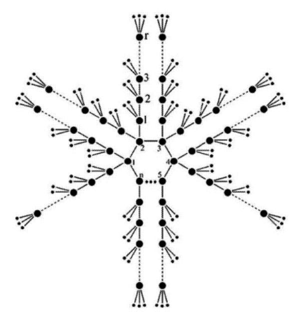

FIGURE 3. Graph model of $C_n^{R_r}$

**Theorem 5.2.** *Let n and r be the positive integers with $n \geq 5$ and $r \geq 2$. Then for a graph $C_n^{R_r}$,*

$$ {}_2M_1(C_n^{R_r}) = 60r(n-1)+30n-46 \text{ and } {}_2M_2(C_n^{R_r}) = 66r(n-1)+60n-112. $$

*Proof.* Let $G = C_n^{R_r}$ and $S = \{\{u,v\} \mid u,v \in V(G) \text{ and } d(u,v)=2\}$. $|V(G)| = 6nr+3n-6r-2$ and $|S| = (2n-2)(6r+3)$. In $G$, there are two vertices of degree 3, $[(n-2)+2r(n-1)]$ vertices of degree 4 and $(4nr-4r+2n-2)$ vertices of degree 1. Then,

$$
\begin{aligned}
{}_2M_1(C_n^{R_r}) &= \sum_{d(u,v)=2} [d_G(u)+d_G(v)] \\
&= 12(4+3)+(2nr-2r+4n-16)(4+4)+4(1+3)+(8nr-8r-2n-2)(1+4) \\
&+(2nr-2r+4n-4)(1+1) \\
&= 60r(n-1)+30n-46
\end{aligned}
$$

and

$$
\begin{aligned}
{}_2M_2(C_n^{R_r}) &= \sum_{d(u,v)=2} d_G(u)d_G(v) \\
&= 12(4\times 3) + (2nr-2r+4n-16)(4\times 4) + 4(1\times 3) + (8nr-8r-2n-2)(1\times 4) \\
&+ (2nr-2r+4n-4)(1\times 1) \\
&= 66r(n-1) + 60n - 112
\end{aligned}
$$

Hence the theorem. □

## 6. On the Chemical Applicability of the Zagreb Indices for $l = 2$

In this section, we will discuss the regression analysis of boiling point (b.p), melting point (m.p), Molar Mass (MM) and density (D) of alkanes on the ${}_2M_1(G)$ and ${}_2M_2(G)$ of the corresponding molecular graph. It is shown that the ${}_2M_1(G)$ and ${}_2M_2(G)$ has a good correlation with boiling point (b.p), melting point (m.p) and Molar Mass (MM) of alkanes.

We have tested the following linear regression model $Y = A + BX$ where $Y$ = dependent physical property, $X$ = topological index .

Using the values presented in Table1, we obtain the following different linear models for each degree based topological index, which are listed below.

**1:** Boiling point (b.p):

$bp = 97.67706 + 2.87081[{}_2M_1(G)]$

$bp = 103.41869 + 2.87081[{}_2M_2(G)]$

**2:** Molar Mass (MM):

$MM = 37.08732 + 3.50664[{}_2M_1(G)]$

$MM = 44.10061 + 3.50664[{}_2M_2(G)]$

**3:** Melting point (m.p):

$m.p = -65.78570 + 1.13488[{}_2M_1(G)]$

$m.p = -63.51593 + 1.13488[{}_2M_2(G)]$

**4:** Density (D):

$D = 0.69998 + 0.00090[{}_2M_1(G)]$

$D = 0.70179 + 0.00090[{}_2M_2(G)]$

| Alkanes | $C_nH_{2n+2}$ | m.p ($°C$) | b.p ($°C$) | MM ($g.mol^{-1}$) | D ($gmL^{-1}$) | ${}_2M_1(G)$ | ${}_2M_2(G)$ |
|---|---|---|---|---|---|---|---|
| Pentane | $C_5H_{12}$ | -129.8 | 36.1 | 72.15 | 0.626 | 10 | 8 |
| Hexane | $C_6H_{14}$ | -95 | 68.8 | 86.18 | 0.660 | 14 | 12 |
| Heptane | $C_7H_{16}$ | -90.5 | 98.38 | 100.20 | 0.679 | 18 | 16 |
| Octane | $C_8H_{18}$ | -56.9 | 125.6 | 114.23 | 0.703 | 22 | 20 |
| Nonane | $C_9H_{20}$ | -53.5 | 150.8 | 128.26 | 0.718 | 26 | 24 |
| Decane | $C_{10}H_{22}$ | -29.7 | 174.1 | 142.29 | 0.730 | 30 | 28 |
| Undecane | $C_{11}H_{24}$ | -25.6 | 195.9 | 156.31 | 0.740 | 34 | 32 |
| Dodecane | $C_{12}H_{26}$ | -9.6 | 216.3 | 170.34 | 0.749 | 38 | 36 |
| Tridecane | $C_{13}H_{28}$ | -5.4 | 235.4 | 184.37 | 0.756 | 42 | 40 |
| Tetradecane | $C_{14}H_{30}$ | 5.9 | 253.5 | 198.39 | 0.763 | 46 | 44 |
| Pentadecane | $C_{15}H_{32}$ | 9.9 | 270.6 | 212.42 | 0.768 | 50 | 48 |
| Hexadecane | $C_{16}H_{34}$ | 18.2 | 286.8 | 226.45 | 0.773 | 54 | 52 |
| Heptadecane | $C_{17}H_{36}$ | 21 | 302 | 240.47 | 0.777 | 58 | 56 |
| Octadecane | $C_{18}H_{38}$ | 29 | 317 | 254.50 | 0.777 | 62 | 60 |
| Nonadecane | $C_{19}H_{40}$ | 33 | 330 | 268.53 | 0.786 | 66 | 64 |
| Icosane | $C_{20}H_{42}$ | 36.7 | 342.7 | 282.55 | 0.789 | 70 | 68 |
| Heneicosane | $C_{21}H_{44}$ | 40.5 | 356.50 | 296.58 | 0.792 | 74 | 72 |
| Docosane | $C_{22}H_{46}$ | 42 | 224 | 310.61 | 0.778 | 78 | 76 |
| Tricosane | $C_{23}H_{48}$ | 49 | 380 | 324.63 | 0.797 | 82 | 80 |
| Tetracosane | $C_{24}H_{50}$ | 52 | 391.3 | 338.66 | 0.797 | 86 | 84 |
| Pentacosane | $C_{25}H_{52}$ | 54 | 401 | 352.69 | 0.801 | 90 | 88 |
| Hexacosane | $C_{26}H_{54}$ | 56.4 | 412.2 | 366.71 | 0.778 | 94 | 92 |
| Heptacosane | $C_{27}H_{56}$ | 59.5 | 422 | 380.74 | 0.780 | 98 | 96 |
| Octacosane | $C_{28}H_{58}$ | 64.5 | 431.6 | 394.77 | 0.807 | 102 | 100 |
| Nonacosane | $C_{29}H_{60}$ | 63.7 | 440.8 | 408.80 | 0.808 | 106 | 104 |
| Triacontane | $C_{30}H_{62}$ | 65.8 | 449.7 | 422.82 | 0.810 | 110 | 108 |
| Hentriacontane | $C_{31}H_{64}$ | 67.9 | 458 | 436.85 | 0.781 | 114 | 112 |
| Dotriacontane | $C_{32}H_{66}$ | 69 | 467 | 450.88 | 0.812 | 118 | 116 |
| Tritriacontane | $C_{33}H_{68}$ | 71 | 474 | 464.90 | 0.811 | 122 | 120 |
| Tetratriacontane | $C_{34}H_{70}$ | 72.6 | 285.4 | 478.93 | 0.812 | 126 | 124 |
| Pentatriacontane | $C_{35}H_{72}$ | 75 | 490 | 492.96 | 0.813 | 130 | 128 |
| Hexatriacontane | $C_{36}H_{74}$ | 75 | 265 | 506.98 | 0.814 | 134 | 132 |
| Heptatriacontane | $C_{37}H_{76}$ | 77 | 504.14 | 520.99 | 0.815 | 138 | 136 |
| Octatriacontane | $C_{38}H_{78}$ | 79 | 510.93 | 535.03 | 0.816 | 142 | 140 |
| Nonatriacontane | $C_{39}H_{80}$ | 78 | 517.51 | 549.05 | 0.817 | 146 | 144 |
| Tetracontane | $C_{40}H_{82}$ | 84 | 523.88 | 563.08 | 0.817 | 150 | 148 |
| Hentetracontane | $C_{41}H_{84}$ | 83 | 530.75 | 577.11 | 0.818 | 154 | 152 |
| Dotetracontane | $C_{42}H_{86}$ | 86 | 536.07 | 591.13 | 0.819 | 158 | 156 |

TABLE 1. The values of boiling point (b.p), melting point (m.p), Molar Mass (MM), density (D), ${}_2M_1(G)$ and ${}_2M_2(G)$ of alkanes

| Parameter | Topological Index | $r$ |
|---|---|---|
| Boiling point | ${}_2M_1(G)$<br>${}_2M_2(G)$ | 0.90395<br>0.90395 |
| Molar Mass | ${}_2M_1(G)$<br>${}_2M_2(G)$ | 1<br>1 |
| Melting point | ${}_2M_1(G)$<br>${}_2M_2(G)$ | 0.90867<br>0.90867 |
| Density | ${}_2M_1(G)$<br>${}_2M_2(G)$ | 0.86054<br>0.86054 |

TABLE 2. The Coefficient Correlation $r$ between topological indices ${}_2M_1(G)$, ${}_2M_2(G)$ and physical properties of alkanes

## 7. CONCLUSION

The first and the second Zagreb index at a distance $l$ which are denoted respectively as ${}_lM_1(G)$ and ${}_lM_2(G)$ are introduced and studied the special case when $l = 2$ in this paper. The lower and the upper bound of ${}_2M_1(G)$, ${}_2M_2(G)$, ${}_2M_1(\overline{G})$ and ${}_2M_2(\overline{G})$ are obtained for any $r$-regular graph $G$. The consistency and the existence of the inverse problem of finding a graph $G$ with prescribed ${}_2M_1(G)$ and ${}_2M_2(G)$ are studied. Finally, the chemical applicability are discussed where a good correlation between boiling point (b.p), melting point (m.p), Molar Mass (MM) with ${}_2M_1(G)$ and ${}_2M_2(G)$ of alkanes are observed.

## ACKNOWLEDGMENT

The authors are very much thankful to the anonymous referee for their suggestions that helped a lot in the improvement of this paper.

## CONFLICT OF INTERESTS

The author(s) declare that there is no conflict of interests.

## REFERENCES

[1] I. Gutman, N. Trinajstic, Graph theory and molecular orbitals. III. Total pi-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972), 535-538.

[2] F. Harary, Graph theory, Narosa Publishing House, New Delhi, 1969.

[3] S. L. Hakimi, On Realizability of a Set of Integers as Degrees of the Vertices of a Linear Graph. I, J. Soc. Ind. Appl. Math. 10 (3) (1962), 496-506.

[4] R.S. Haoer, K.A. Atan, A.M. Khalaf, M.R. Md. Said and R. Hasni, Eccentric Connectivity Index of Certain Classes of Cycloalkenes, Proceedings of the International Conference on Computing, Mathematics and Statistics (iCMS 2015), Springer Nature Singapore Pte Ltd. (2017), 235-242.

[5] A. Rizwana, G. Jeyakumar and S. Somasundaram, On Non-Neighbor Zagreb Indices and Non-Neighbor Harmonic Index, Int. J. Math. Appl. 4 (2016), 89-101.

[6] G. R. Roshini and S. B. Chandrakala, Multiplicative Zagreb Indices of Transformation Graphs, Anusandhana J. Sci. Eng. Manage. 6 (1) (2018), 18-30.

[7] G. R. Roshini, S. B. Chandrakala and B. Sooryanarayana, Some degree based topological indices of transformation graphs, Bull. Int. Math. Virtual Inst. 10 (2) (2020), 225-237.

[8] B. Sooryanarayana, S. B. Chandrakala and G. R. Roshini, On Realization and Characterization of Topological Indices, Int. J. Innovat. Technol. Explor. Eng. 9 (1) (2019), 715-718.