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# ON THE EXTREMAL GRAPHS FOR SECOND ZAGREB INDEX WITH FIXED NUMBER OF VERTICES AND CYCLOMATIC NUMBER

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*Abstract.* The cyclomatic number of a graph $G$ (is denoted by $\nu$) is the minimum number of edges of $G$ whose removal makes $G$ as acyclic. Denote by $\mathbb{G}_{n,\nu}$ the collection of all $n$-vertex connected graphs with cyclomatic number $\nu$. The elements of $\mathbb{G}_{n,\nu}$ with maximum second Zagreb ($M_2$) index (for $\nu \leq 4$ and $\nu = \frac{k(k-3)}{2} + 1$, where $4 \leq k \leq n-2$) and with minimum $M_2$ index (for $\nu \leq 2$) have already been reported in the literature. The main contribution of the present article is the characterization of graphs in the collection $\mathbb{G}_{n,\nu}$ with minimum $M_2$ index for $\nu \geq 3$ and $n \geq 2(\nu-1)$. The obtained extremal graphs, are molecular graphs and thereby, also minimize $M_2$ index among all the connected molecular $n$-vertex graphs with cyclomatic number $\nu \geq 3$, where $n \geq 2(\nu-1)$. For $n \geq 6$, the graph having maximum $M_2$ value in the collection $\mathbb{G}_{n,5}$ has also been characterized and thereby a conjecture posed by Xu *et al.* [*MATCH Commun. Math. Comput. Chem.* **72** (2014) 641–654] is confirmed for $\nu = 5$.

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## 1. INTRODUCTION

All the graphs considered in the present study are finite, undirected, simple and connected. Undefined notations and terminologies from (chemical) graph theory can be found in [11, 24].

Chemical compounds can be represented by graphs in which vertices correspond to the atoms while edges represent the covalent bonds between atoms [24]. In chemical graph theory, graph invariants are usually referred as *topological indices*. In 1972, Gutman and Trinajstić [9] showed that total $\pi$-electron energy of a molecule $M$ depends on the topological index $\sum_{v \in V(G)} d_v^2$, where $G$ is the graph corresponding to $M$, $V(G)$ is the vertex set of $G$ and $d_v$ is degree of the vertex $v$. Nowadays, this graph quantity is known as the *first Zagreb index* and is denoted by $M_1$. The following topological index (currently known as *second Zagreb index* and is usually denoted by

$M_2$) was appeared in [8] within the study of molecular branching:

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where $E(G)$ is the edge set of the graph $G$ and $uv$ is the edge between the vertices $u, v \in V(G)$. Both of the aforementioned Zagreb indices belong to the oldest and most studied topological indices. More than five hundred papers have been devoted to these Zagreb indices, for example see the reviews [4,7,21] published on the occasion of their 30th anniversary, recent surveys [2,6], recent papers [3,12–18,20,22,23] and related references mentioned therein.

A vertex $v \in V(G)$ is said to be pendent vertex if $d_v = 1$. Following Xu *et al.* [25], let $K_k^{n-k}$ be the graph obtained by attaching $n-k$ pendent vertices to one vertex of the $k$-vertex complete graph $K_k$. For any positive integer $t < k$, let $K_k^{n-k}(t)$ be a graph obtained by adding $t$ new edges between one pendent vertex of $K_k^{n-k}$ and $t$ vertices with degree $k-1$ in it. The cyclomatic number of a graph $G$ (is denoted by $\nu$) is the minimum number of edges of $G$ whose removal makes $G$ as acyclic. Denote by $\mathbb{G}_{n,\nu}$ the collection of all $n$-vertex connected graphs with cyclomatic number $\nu$. Even though the mathematical theory of Zagreb indices is well established, some important extremal graph-theoretical problems concerning these Zagreb indices are still open. One of these problems is the characterization of extremal graphs with respect to $M_2$ index in $\mathbb{G}_{n,\nu}$ (however, a similar problem concerning $M_1$ index has already been solved completely [25]). Indeed, partial solution of the aforementioned problem (for $M_2$ index) has been reported in the literature: see [5] for the characterization of graphs in $\mathbb{G}_{n,\nu}$ with minimum $M_2$ value in case of $\nu \leq 2$; see [5] for the characterization of graphs in $\mathbb{G}_{n,\nu}$ with maximum $M_2$ value in case of $\nu \leq 2$ and $\nu = 4$, respectively. Also, Xu *et al.* [25] characterized the members of $\mathbb{G}_{n,\nu}$ with maximum $M_2$ value for $\nu \leq 3$ and $\nu = \frac{k(k-3)}{2} + 1$, where $4 \leq k \leq n-2$. Furthermore, the authors of [25] posed the following conjecture concerning maximum $M_2$ value:

**Conjecture 1.** *Let* $\nu = \frac{k(k-3)}{2} + t + 1$ *where* $1 \leq t \leq k-1$ *and* $4 \leq k \leq n-2$. *The graph* $K_k^{n-k}(t)$ *attains maximum* $M_2$ *value among all the members of* $\mathbb{G}_{n,\nu}$.

For $\nu = 4$, the Conjecture 1 was proved in [1, 10]. In this paper, we confirm the Conjecture 1 for $\nu = 5$ and, mainly, characterize the graphs with minimum $M_2$ value in the collection $\mathbb{G}_{n,\nu}$ for $\nu \geq 3$ and $n \geq 2(\nu - 1)$.

## 2. Main Results

In order to obtain the main results, we need to establish some preliminary lemmas and thereby we recall some notations and definitions. For a vertex $u \in V(G)$, the set of all vertices adjacent with $u$ is denoted by $N_G(u)$. The elements of $N_G(u)$ are called neighbors of $u$. A vertex $v \in V(G)$ is said to be branching vertex if $d_v \geq 3$. A path $v_1 v_2 \cdots v_{k+1}$ of length $k \geq 1$ in a graph $G$ is said to be pendent path if one of the vertices $v_1$, $v_{k+1}$ is branching and the other one is pendent, and all the other vertices (if exist) $v_2, v_3, \ldots, v_k$ of path have degree 2. Let $G'$ be a graph obtained from another graph $G$ by applying some graph transformation such that $V(G) = V(G')$. In the rest of the paper, whenever such two graphs are under discussion, by the vertex degree $d_u$ we always mean the degree of the vertex $u$ in $G$.

**Lemma 1.** *For $\nu \geq 3$ and $n \geq 2(\nu - 1)$, if $G$ has minimum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$ then $G$ does not contain any pendant vertex.*

*Proof.* Suppose to the contrary that $G$ has a pendent vertex. Let $uu_1u_2 \ldots u_r$ be a pendent path in $G$, where $d_u \geq 3$. Assume that $v$ is a neighbor of $u$ different from $u_1$. Let $G'$ be the graph obtained from $G$ by removing the edge $uv$ and adding the edge $vu_r$. We note that both the graphs $G$ and $G'$ have same cyclomatic number. If $r = 1$ then

$$\begin{aligned} M_2(G) - M_2(G') &= d_v(d_u - 2) - d_u + 2 + \sum_{x \in N_G(u): x \neq u_1, x \neq v} d_x \\ &\geq d_v - d_u + 2 + \sum_{x \in N_G(u): x \neq u_1, x \neq v} d_x > 0, \end{aligned}$$

which is a contradiction to the minimality of $M_2(G)$. If $r \geq 2$ then we have

$$M_2(G) - M_2(G') = d_v(d_u - 2) + \sum_{x \in N_G(u): x \neq u_1, x \neq v} d_x \geq d_v + \sum_{x \in N_G(u): x \neq u_1, x \neq v} d_x > 0,$$

again a contradiction. □

Let $n_i$ be the number of vertices of degree $i$ in the graph $G$. The minimum and maximum vertex degree of a graph is denoted by $\delta$ and $\Delta$ respectively.

**Lemma 2.** *For $\nu \geq 3$ and $n \geq 2(\nu - 1)$, if $G$ has minimum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$ then maximum vertex degree in $G$ is 3.*

*Proof.* From Lemma 1, we have $\delta \geq 2$. The assumption $\nu \geq 3$ and the fact that the $n$-vertex cycle graph $C_n$ is the only connected graph for which minimum and maximum vertex degree is 2, implies that maximum vertex degree in $G$ is at least 3. We have to show that $\Delta = 3$. Contrarily, suppose that $\Delta \geq 4$. The inequality $n \geq 2(\nu - 1)$ implies that

$$\sum_{2 \leq i \leq \Delta} n_i \geq 2(m - n) = 2\left(\sum_{2 \leq i \leq \Delta} \frac{in_i}{2} - \sum_{2 \leq i \leq \Delta} n_i\right) = 2\left(\sum_{3 \leq i \leq \Delta} \frac{in_i}{2} - \sum_{3 \leq i \leq \Delta} n_i\right),$$

which is equivalent to

$$n_2 \geq \sum_{4 \leq i \leq \Delta} (i - 3)n_i.$$

It means that $G$ contains at least one vertex of degree 2. Suppose that the vertex $u \in V(G)$ has maximum degree.

*Case 1.* The vertex $u$ has a neighbor $w$ of degree 2.
We note that $w$ is not adjacent to at least one neighbor, say $v$, of $u$. Let $G'$ be the graph obtained from $G$ by removing the edge $uv$ and adding the edge $vw$. Then, we have $M_2(G) - M_2(G') > 0$, a contradiction because $\delta \geq 2$ and

$$M_2(G) - M_2(G') = d_v(d_u - 3) - d_t - d_u + 3 + \sum_{x \in N_G(u); x \neq v, x \neq w} d_x$$
$$\geq 2(d_u - 3) - d_t - d_u + 3 + \sum_{x \in N_G(u); x \neq v, x \neq w} d_x,$$

where $t$ is the neighbor of $w$ different from $u$.
*Case 2.* All the neighbors of $u$ have degree greater than 2.
We notice that there exists a vertex $w' \in V(G) \setminus N_G(u)$ of degree 2 which is not adjacent to at least one neighbor, say $v'$, of $u$. Let $G''$ be the graph obtained from $G$ by removing the edge $uv'$ and adding the edge $v'w'$. Due to the assumption $d_u = \Delta \geq 4$, we have

$$M_2(G) - M_2(G'') = d_{v'}(d_u - 3) + \sum_{y \in N_G(u): y \neq v'} d_y - \sum_{z \in N_G(w')} d_z$$
$$\geq 3(d_u - 3) + 3(d_u - 1) - 2d_u > 0,$$

again a contradiction. This completes the proof. ☐

Let $x_{i,j}$ be the number of edges in the graph $G$ connecting the vertices of degrees $i$ and $j$.

**Lemma 3.** *For $\nu \geq 3$, let $G \in \mathbb{G}_{n,\nu}$ such that it contains only vertices of degree 2 and 3.*

(i) *If $2(\nu - 1) \leq n < 5(\nu - 1)$ then at least two vertices of degree 3 are adjacent.*
(ii) *If $n > 5(\nu - 1)$ then at least two vertices of degree 2 are adjacent.*
(iii) *If $n = 5(\nu - 1)$ and if one of $x_{2,2}, x_{3,3}$ is zero then the other is also zero.*

*Proof.* $(i)$ From the definition of $G$, the following equations must holds:

$$n_2 + n_3 = n \quad (2.1)$$
$$2n_2 + 3n_3 = 2(n + \nu - 1) \quad (2.2)$$
$$2x_{2,2} + x_{2,3} = 2n_2 \quad (2.3)$$
$$x_{2,3} + 2x_{3,3} = 3n_3. \quad (2.4)$$

From Eqs. (2.1) and (2.2), we obtain $n_2 = n - 2(\nu - 1)$ and $n_3 = 2(\nu - 1)$. These two equations together with the assumption $n < 5(\nu - 1)$ imply that

$$2n_2 < 3n_3. \quad (2.5)$$

If $x_{3,3} = 0$ then from Eqs. (2.3) and (2.4), it follows that $2n_2 \geq 3n_3$ which contradicts the Inequality (2.5). From this we conclude that at least two vertices of degree 3 are adjacent.

(ii) The proof is fully analogous to that of first part.
(iii) The assumption $n = 5(\nu - 1)$ implies that $2n_2 = 3n_3$. Now, from Eqs. (2.3) and (2.4), the desired result follows.

□

**Lemma 4.** *For $\nu \geq 3$ and $n > 5(\nu - 1)$, if $G$ has minimum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$ then for every edge $xy \in E(G)$ at least one of the vertices $x, y$ has degree 2.*

*Proof.* From Lemmata 1, 2 and 3, it follows that $G$ contains only vertices of degrees 2, 3 and contains at least two adjacent vertices of degree 2, say $u$ and $v$. Suppose to the contrary that there exist two adjacent vertices $w, t \in V(G)$ of degree 3. Let $x \neq u$ be the vertex adjacent with $v$. The vertex $x$ may coincides with $w$ or $t$, if this is the case, then (without loss of generality) we may assume that $x = t$.
*Case 1.* The vertices $u$ and $v$ do not have common neighbor.
Let $G'$ be the graph obtained from $G$ by removing the edges $uv, vx, wt$ and adding the edges $ux, wv, tv$. Whether $x = t$ or $x \neq t$, in both the cases, we have $M_2(G) - M_2(G') = 1$, a contradiction to the minimality of $M_2(G)$.
*Case 2.* The vertices $u$ and $v$ have common neighbor.
It is evident that $d_x = 3$. If $x \neq t$ then the graph $G''$ obtained from $G$ by removing the edges $vx, wt$ and adding the edges $vt, wx$, has same $M_2$ value as $G$ has. The vertices $u$ and $v$ do not have common neighbor in the graph $G''$ and hence by Case 1, we arrives at a contradiction. If $x = t$ then we consider a neighbor $w_1$ of $w$ different from $t$. If $G'''$ is the graph obtained from $G$ by removing the edges $vt, w_1w$ and adding the edges $wv, w_1t$, then $M_2(G) = M_2(G''')$. Again, the vertices $u$ and $v$ do not have common neighbor in the graph $G'''$ and hence by Case 1, we arrives at a contradiction. □

**Lemma 5.** *For $\nu \geq 3$ and $n = 5(\nu - 1)$, if $G$ has minimum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$ then for every edge $xy \in E(G)$ one of the vertices $x, y$ has degree 2 and the other has degree 3.*

*Proof.* From Lemmas 1 and 2, it follows that $G$ contains only vertices of degree 2 and 3. We claim that $x_{2,2} = x_{3,3} = 0$. Contrarily, suppose that at least one of $x_{2,2}, x_{3,3}$ is non-zero. If one of $x_{2,2}, x_{3,3}$ is zero then (due to Lemma 3) the other must also be zero, a contradiction. If both of $x_{2,2}, x_{3,3}$ are non-zero. Then, from the proof of Lemma 4, we conclude that there exists a graph $G' \in \mathbb{G}_{n,\nu}$ such that $M_2(G) > M_2(G')$, which is again a contradiction.

□

**Lemma 6.** *For $\nu \geq 3$ and $2(\nu - 1) \leq n < 5(\nu - 1)$, if $G$ has minimum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$ then $G$ does not contain any edge connecting the vertices of degree 2.*

*Proof.* Contrarily, suppose that $G$ contains at least two adjacent vertices of degree 2, say $u$ and $v$. From Lemmas 1, 2 and 3, it follows that $G$ has at least two adjacent vertices of degree 3. From the proof of Lemma 4, we conclude that there exists a graph $G' \in \mathbb{G}_{n,\nu}$ such that $M_2(G) > M_2(G')$, which is a contradiction. □

**Theorem 1.** *If* $\nu \geq 3$ *then among all the members of* $\mathbb{G}_{n,\nu}$*,*

(i) *the cubic graphs uniquely attains minimum* $M_2$ *value (which is* $9(\nu+n-1)$*) for* $n = 2(\nu-1)$*;*

(ii) *the graphs containing only vertices of degree 2 and 3 such that no two vertices of degree 2 are adjacent, uniquely attain minimum* $M_2$ *value (which is* $3n+21(\nu-1)$*) for* $2(\nu-1) < n < 5(\nu-1)$*;*

(iii) *the graphs containing only vertices of degree 2 and 3 such that for every pair of adjacent vertices of G one vertex has degree 2 and the other vertex has degree 3, uniquely attain minimum* $M_2$ *value (which is* $6(\nu+n-1)$*) for* $n = 5(\nu-1)$*;*

(iv) *the graphs containing only vertices of degree 2 and 3 such that no two vertices of degree 3 are adjacent, uniquely attain minimum* $M_2$ *value (which is* $4n+34(\nu-1)$*) for* $n > 5(\nu-1)$.

*Proof.* Let $G \in \mathbb{G}_{n,\nu}$ be the graph with minimum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$. From Lemmas 1 and 2, it is concluded that $G$ contains only vertices of degree 2 and 3.

(i) If $n = 2(\nu-1)$ then Eqs. (2.1) and (2.2) yield $n_2 = 0$ and hence $G$ must be a cubic graph.

(ii) If $2(\nu-1) < n < 5(\nu-1)$ then bearing in mind the Lemma 6, we find the values of $x_{2,3}$, $x_{3,3}$ from Eqs. (2.1) - (2.4): $x_{2,3} = 2(n-2(\nu-1))$, $x_{3,3} = 5(\nu-1)-n$. Hence $M_2(G) = 3n+21(\nu-1)$.

(iii) A direct consequence of Lemma 5.

(iv) If $n > 5(\nu-1)$ then bearing in mind the Lemma 4 we find the values of $x_{2,2}$, $x_{2,3}$ from Eqs. (2.1) - (2.4): $x_{2,2} = n-5(\nu-1)$, $x_{2,3} = 6(\nu-1)$. Hence $M_2(G) = 4n+34(\nu-1)$.

□

*Remark* 1. We note that all the extremal graphs characterized in Theorem 1 are molecular graphs. Hence, these extremal graphs also minimize $M_2$ among all the (connected) molecular $n$-vertex graphs with cyclomatic number $\nu \geq 3$, where $n \geq 2(\nu-1)$.

*Remark* 2. If a graph $G \in \mathbb{G}_{n,\nu}$ has size $m$ then it holds $\nu = m-n+1$ and thereby the extremal values mentioned in Theorem 1 can be rewritten in terms of order and size of the graph.

Miličević *et al.* [19] reformulated the first Zagreb index in terms of edge-degrees instead of vertex-degrees. This topological index is denoted by $EM_1$ and can be defined as:

$$EM_1(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)^2.$$

*Remark* 3. We remark that the graphs which minimize $M_2$ index among all the members of the collection $\mathbb{G}_{n,\nu}$ (where $\nu \geq 3$), also minimize $EM_1$ index in the aforementioned collection. We omit details because the proofs of the results corresponding to Lemmas 1, 2, Lemma 4 - Lemma 6 and Theorem 1 concerning $EM_1$ index are fully analogous to that of Lemmas 1, 2, Lemma 4 - Lemma 6 and Theorem 1.

Since all the extremal graphs in Theorem 1 have minimum degree 2, we derive a sharp lower bound on $M_2$ for the $n$-vertex graph with minimum degree at least 2 and cyclomatic number $\nu$.

**Theorem 2.** *If $G$ is an $n$-vertex graph with minimum degree at least 2 and cyclomatic number $\nu$ then $M_2(G) \geq 29(\nu - 1) - n$ with equality if and only if $G$ is cubic graph.*

*Proof.* Bearing in mind the equations

$$M_2(G) = \sum_{2 \leq i \leq j \leq \Delta} ij.x_{i,j} \ ,$$

$$\nu + n - 1 = \sum_{2 \leq i \leq j \leq \Delta} x_{i,j} \ ,$$

$$n = \sum_{2 \leq i \leq j \leq \Delta} \left( \frac{1}{i} + \frac{1}{j} \right) x_{i,j} \ ,$$

we have

$$M_2(G) - 29(\nu + n - 1) + 30n = \sum_{2 \leq i \leq j \leq \Delta} \left( ij - 29 + \frac{30}{i} + \frac{30}{j} \right) x_{i,j}.$$

To obtain the desired result, we have to show that $f(i,j) = ij - 29 + \frac{30}{i} + \frac{30}{j} \geq 0$ for $2 \leq i \leq j \leq \Delta$ such that $f(i,j) = 0$ if and only if $i = j = 3$. Direct calculations yield $f(2,j) > 0$ for $j = 2,3$. For all $j \geq 4$, it holds that $f(2,j) \geq f(2,4) > 0$. Also, we note that $f(3,3) = 0$ and $f(3,j) \geq f(3,4) > 0$ for all $j \geq 4$. Finally, if $j \geq i \geq 4$ then extension of the function $f$ to the interval $[4,\infty)$ is increasing in both variables and hence $f(i,j) \geq f(4,4) > 0$. This completes the proof. □

Now, we turn our attention to the prove the Conjecture 1 for $\nu = 5$. For this, we need the following useful lemma:

**Lemma 7.** [25] *If the graph $G$ has maximum $M_2$ value among all the members of $\mathbb{G}_{n,\nu}$ then the maximum vertex degree in $G$ is $n - 1$.*

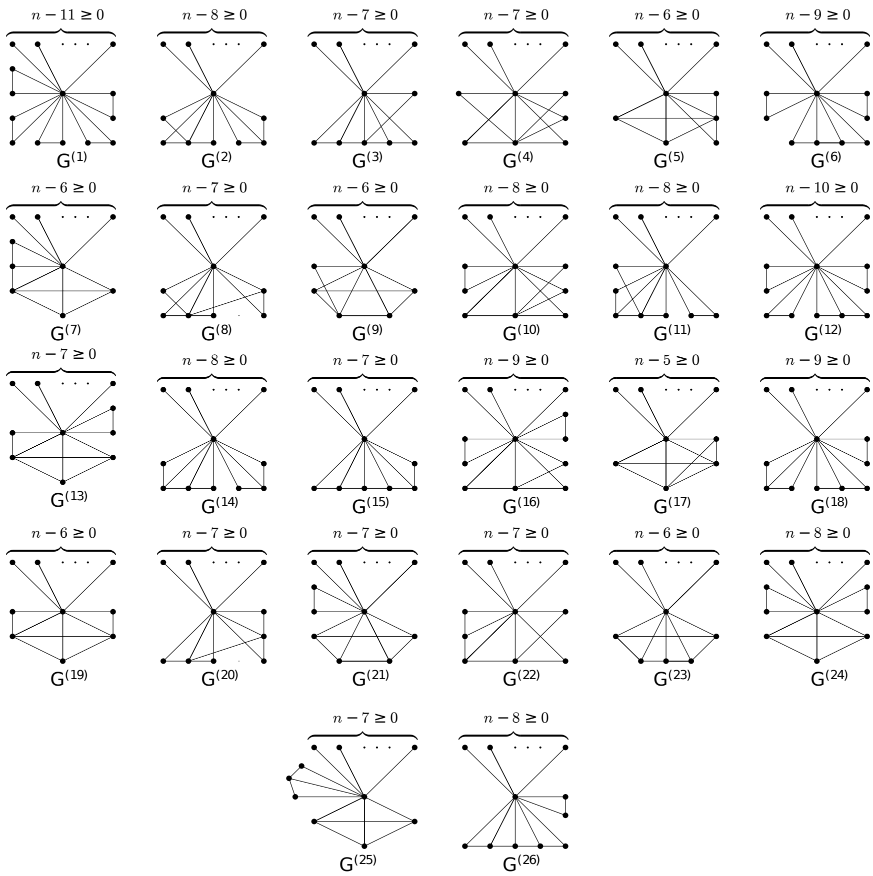


FIGURE 1. All the non-isomorphic graphs in $\mathbb{G}_{n,5}$ with maximum degree $n-1$.

**Theorem 3.** *For $n \geq 6$, the graph $G^{(17)}$ (which is isomorphic to $K_4^{n-4}(2)$ and is depicted in Figure 1) uniquely maximizes $M_2$ among all the members of $\mathbb{G}_{n,5}$, where $M_2(G^{(17)}) = n^2 + 8n + 55$.*

*Proof.* Firstly, we enumerate all the non-isomorphic members of $\mathbb{G}_{n,5}$ having maximum vertex degree $n-1$, which can be obtained from the $n$-vertex star graph $S_n$ by adding five (possible) edges. All these non-isomorphic graphs are shown in Figure 1. From Lemma 7, it follows that the member of $\mathbb{G}_{n,\nu}$ which maximize $M_2$ must be one of the graphs $G^{(1)}, G^{(2)}, \ldots, G^{(26)}$. Let $a_1 = 11, a_2 = 27, a_3 = a_{10} = 35, a_4 = 51, a_5 = 50, a_6 = 20, a_7 = a_8 = 42, a_9 = 41, a_{11} = 29, a_{12} = 15, a_{13} = a_{23} = 36, a_{14} = 24, a_{15} = a_{25} = 30, a_{16} = 23, a_{17} = 55, a_{18} = 19, a_{19} = 47, a_{20} = 39, a_{21} = 31, a_{22} = 34, a_{24} = 26, a_{26} = 25$. Routine calculations yield $M_2(G^{(i)}) = n^2 + 8n + a_i$, where $i = 1, 2, 3, \ldots, 26$. Simple comparison gives the desired result. □

## 3. Concluding remarks

We have characterized the graphs having minimum $M_2$ value among all the $n$-vertex connected graphs (and molecular graphs) with cyclomatic number $\nu \geq 3$, where $n \geq 2(\nu - 1)$. We have also characterized the graphs having maximum $M_2$ value among all the $n$-vertex connected graphs with cyclomatic number $\nu = 5$ and thereby confirmed the Conjecture 1 for $\nu = 5$. We believe that this conjecture is true. However, at the present moment, we do not have its proof.

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