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Which Valence Connectivities Realize Monocyclic Molecules: Generating Algorithm and Its Application to Test Discriminative Properties of the Zagreb and Modified Zagreb Indices

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Valence connectivities in hydrogen suppressed graphs are characterized by 10-tuples of quantities m_{ij} where m_{ij} is the number of edges that connect vertices of valences i and j. It is shown which 10-tuples are realizable by monocyclic graphs and this finding is used to compare discriminative properties of the Zagreb and modified Zagreb indices.

INTRODUCTION

Connectivity of atoms in the molecule is conveniently described by the corresponding molecular graph. The atoms are represented by vertices and bonds by edges of graphs. Such approach enables one to relate properties of molecules to their connectivities and has been a subject of intensive research in the last few decades.[1,2]

Molecular graphs can be numerically characterized in a variety of ways. The simplest numbers ascribed to a graph are the number of its vertices and its edges. Each vertex x in a given graph G can be characterized by the number of its neighboring vertices, $d_G(x)$, which is called a vertex degree and which obviously parallels the chemical notion of the valence of atoms.

Connectivity of vertices in a graph can be further characterized by specifying the numbers m_{ij} of edges that connect (adjacent) vertices of degrees i and j. Obviously, the unique sequence of m_{ij}s is ascribed to any graph, but the opposite generally does not hold, *e.g.* there is no graph with $m_{12} = 1$ and all other m_{ij} being equal to zero.

This nontrivial problem has been recently attacked in a series of papers. Firstly, the problem of the existence of graphs with a given sequence of m_{ij}s for $i, j = 1,2,4$ was solved[3] and after that it was generalized for $i, j = 1,2,3,4$.[4] The algorithms obtained are rather involved, but for special classes of graphs one should hope to develop particular and faster algorithms. Indeed, such an algorithm was developed for connected acyclic graphs (trees) with $i, j = 1,2,3,4$.[5]

In this paper, monocyclic graphs, *i.e.* connected graphs having only one cycle and an arbitrary number of trees attached to it are studied.

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In the second section basic definitions and notations are introduced and in the third section necessary and sufficient conditions of m_{ij}s for the existence of monocyclic graph(s) are determined. These conditions are summarized in Theorem 5. Based on this theorem and Theorems 6–8, an efficient generating algorithm is developed that gives all m_{ij} sequences corresponding to monocyclic graphs with a given number of vertices. Finally, in the fifth section, this algorithm is utilized to test discriminative properties of the Zagreb and modified Zagreb indices in monocyclic graphs.

PRELIMINARIES

Here we consider connected graphs with the maximal degree at most 4 and with a finite number of vertices. Further, we restrict our attention to monocyclic graphs, *i.e.* to the graphs having only one cycle. The set of all monocyclic graphs is denoted by T.

To each graph G∈T a unique sequence

$$(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$$

can be associated in such a way that in graph G there are exactly m_{ij} edges that are adjacent with vertices of degrees i and j. In this way, a function μ:T$\rightarrow N_0^{10}$ is defined, where N_0^{10} is the set of all 10-tuples of nonnegative integers (*i.e.* $N_0 = N \cup \{0\}$, where N is the set of natural numbers). It can be easily seen that this function is not a surjection (or mapping onto), *e.g.* there is no graph G∈T such that $m_{11} = 4$ and $m_{12} = m_{13} = m_{14} = m_{22} = m_{23} = m_{24} = m_{33} = m_{34} = m_{44} = 0$.

Therefore, it is of interest for chemistry to find a necessary and sufficient condition for an arbitrary sequence $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$ to belong to the set μ(T). In the second section, we find these necessary and sufficient conditions.

The following equation: $m_{11} + m_{12} + m_{13} + m_{14} + m_{22} + m_{23} + m_{24} + m_{33} + m_{34} + m_{44} = n$ holds for monocyclic graphs with n vertices. In the fourth section, we use the result of the previous sections to find a fast algorithm that generates all the sequences $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in \mu$ for prescribed $n = \sum m_{ij} \in N$ (T).

Note that if we try to derive these sequences $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$ explicitly, we would need to construct all trees with maximal degrees smaller than or equal to 4. It can be easily shown that this is a nonpolynomial problem. Using our theorems, we can generate these sequences in polynomial time. This is a key feature of our algorithm, because one of the most important goals of theoretical computer science is to replace as many nonpolynomial algorithms as possible by polynomial ones.

This algorithm promises important chemical applications, *e.g.* as explained in the fifth section, it enables a comparison of discriminative properties of the Zagreb and modified Zagreb indices.

57 years ago, chemists[6] noticed that information given by a graph can be compressed in a single number, the so called molecular descriptor. Of course, there is an infinite number of ways to do this and only those descriptors which correlate well with physical, chemical and biological properties of molecules are of interest. These indices, the so called topological inidices, have found enormous applications in QSPR (Quantitive Structure Property Relationship) and QSAR (Quantitive Structure Activity Relationship) and other studies, and the reader is referred to recent monographs for an overview.[7,8] Many of these indices are uniquely defined by a sequence (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}). A well known such index is the Zagreb index[9] defined by

$$M_2(\mathrm{G}) = \sum_{\{x,y\}\in E(\mathrm{G})} d_\mathrm{G}(x)\, d_\mathrm{G}(y) = \sum_{1\le i\le j\le 4} i \cdot j \cdot \mu_{ij}(\mathrm{G}),$$

where μ_{ij}(G) denotes the number of edges that connect vertices of degree i and degree j. Properties and applications of this index and its relationship with other topological indices have been recently reviewed.[10]

The following modification of the Zagreb index, the so called modified Zagreb index, is proposed:[10,11]

$$^*M_2(\mathrm{G}) = \sum_{\{x,y\}\in E(\mathrm{G})} \frac{1}{d_\mathrm{G}(x)\, d_\mathrm{G}(y)} = \sum_{1\le i\le j\le 4} \frac{\mu_{ij}(\mathrm{G})}{ij}$$

Obviously, if two graphs G and G' have equal sequences μ(G) and μ(G'), they cannot be discriminated by any of the two above indices. On the other hand, one or/and the other of these indices can be the same for nonequal sequences. Using the algorithm developed in the fourth section, in the fifth section we analyze how well these indices distinguish sequences $m,m' \in \mu$(T).

Herein, we use the standard graph theory terms and notations. Let G be a graph with vertex set V(G) and edge set E(G). Let $A,B \subseteq V$(G) where A and B are disjoint sets. By G[A] we denote the subgraph of G induced by the vertex set A, by $E_\mathrm{G}(A)$ we denote the set of edges of G with both adjacent vertices in A, by $E_\mathrm{G}(A,B)$ we denote the set of edges of G with one adjacent vertex in A and the other in B. We also put $e_\mathrm{G}(A) = |E_\mathrm{G}(A)|$ and $e_\mathrm{G}(A,B) = |E_\mathrm{G}(A,B)|$. Let G be a graph and S a set of edges in complement of G. By G + S we denote the graph obtained from G by adding the set S.

We also define functions μ_{ij}: T$\rightarrow N_0$, for each $1 \le i \le j \le 4$ by $\mu_{ij}(\mathrm{G}) = m_{ij}$ if and only if exactly m_{ij} edges connect vertices with degrees i and j in graph G. Also by A_n we denote the set of all monocyclic graphs with n vertices having the maximal degree at most 4.

The edge connecting vertex with itself is called a loop and the pair of edges having the same terminal vertices are called parallel edges. At the end of this section, we give the following definition:

Definition 1. – Let $p,q,r \in N_0$ and $n_3,n_4 \in N$ such that $p+q+r = n_3+n_4$. Set F (n_3, n_4, p, q, r) is the set of graphs G such that $V(G) = N_3 \cup N_4$; $N_3 = \{x_1,\ldots, x_{n_3}\}$; $N_4 = \{y_1, y_2\ldots, y_{n_4}\}$; $e_G(N_3) = p$; $e_G(N_3, N_4) = q$; $e_G(N_4) = r$; $d_G(x) \leq 3$, for each $x \in N_3$; and $d_G(y) \leq 4$, for each $y \in N_4$. Further, G is a simple graph except in the following cases in which it has one of the following: a single loop or a single pair of parallel edges:

1) $(n_3 = 1)$ and $(p = 1)$. There is a single loop adjacent to x_1.
2) $(n_4 = 1)$ and $(r = 1)$. There is a single loop adjacent to y_1.
3) $(n_3 = 2)$ and $(p = 2)$. There is a pair of parallel edges adjacent to x_1 and x_2.
4) $(n_4 = 2)$ and $(r = 2)$. There is a pair of parallel edges adjacent to y_1 and y_2.
5) $(n_3 = 1)$ and $(p = 0)$ and $(r = 0)$. There is a pair of parallel edges adjacent to x_1 and y_1.
6) $(n_4 = 1)$ and $(p = 0)$ and $(r = 0)$. There is a pair of parallel edges adjacent to x_1 and y_1.

Set F (n_3, n_4, p, q, r) is the auxiliary family of graphs that will be needed to obtain further results.

NECESSARY AND SUFFICIENT CONDITIONS OF VALENCE CONNECTIVITIES FOR THE EXISTENCE OF A MONOCYCLIC MOLECULAR GRAPH

In this section, we give a mathematical background of the algorithm that will be developed in the next section, *i.e.* we give the necessary and sufficient conditions of m_{ij} for the existence of a monocyclic molecular graph. We start with few lemmas:

Lemma 2. – Let $k,l \in \mathbb{N}$ and let $a_1,a_2,\ldots,a_k, b_1,\ldots,b_l \in N_0$ and let

$$\max\{b_1,\ldots,b_l\} - \min\{b_1,\ldots,b_l\} \leq 1$$

$$q \leq \min\left\{\sum_{i=1}^{k} \min\{a_i, l\}, \sum_{i=1}^{l} b_i\right\},$$

then there is a simple bipartite graph G with q edges and partition classes $A = \{x_1,\ldots,x_k\}$ and $B = \{y_1,\ldots,y_l\}$ such that $d_G(x_i) \leq a_i$ for each $i = 1,\ldots,k$ and $d_G(y_i) \leq b_i$ for each $i = 1,\ldots,l$.

Proof. We prove the claim by induction on k. If $k = 1$, then the claim is trivial. Let us prove the inductive step. Distinguish three cases:

$$1)\ \min\left\{l, d_G(a_k), \sum_{i=1}^{l} b_i\right\} = l.$$

In this case, we have $q - l \leq \min\left\{\sum_{i=1}^{k-1} \min\{a_i, l\}, \sum_{i=1}^{l} b_i - 1\right\}$, therefore there is, by inductive hypothesis, a bipartite graph G' with partition classes $\{a_1,\ldots,a_{k-1}\}$ and B such that $d_G(x_i) \leq a_i$ for each $i = 1,\ldots,k-1$ and $d_G(y_i) \leq b_i - 1$ for each $i = 1,\ldots,l$. Graph $G = G' + \{a_kb_1,\ldots,a_kb_l\}$ has the required properties.

$$2)\ \min\left\{l, d_G(a_k), \sum_{i=1}^{l} b_i\right\} = d_G(a_k).$$

Without loss of generality, we may assume that $b_1 \geq b_2 \geq \ldots \geq b_l$. In this case, we have

$$\max\{b_1-1,\ldots, b_{d_G(x_k)}-1, b_{d_G(x_k)+1},\ldots,b_l\} - \min\{b_1-1,\ldots, b_{d_G(x_k)}-1, b_{d_G(x_k)+1},\ldots,b_l\} \leq 1;$$

$$q - d_G(a_k) \leq \min\left\{\sum_{i=1}^{k-1} \min\{a_i, l\}, \sum_{i=1}^{d_G(x_k)} b_i - 1 + \sum_{i=d_G(x_k)+1}^{l} b_i\right\},$$

and therefore there exists, by inductive hypothesis, a bipartite graph G' with partition classes $\{a_1,\ldots,a_{k-1}\}$ and B such that $d_G(x_i) \leq a_i$ for each $i = 1,\ldots,k-1$, and $d_G(y_i) \leq b_i - 1$ for each $i = 1,\ldots, d_G(x_k)$, and $d_G(y_i) \leq b_i$ for each $i = d_G(x_k) + 1,\ldots,l$. Graph $G = G' + \{a_kb_1,\ldots, a_kb_{d_G(x_k)}\}$ has the required properties.

$$3)\ \min\left\{l, d_G(a_k), \sum_{i=1}^{l} b_i\right\} = \sum_{i=1}^{l} b_i.$$

This case is trivial.

Lemma 3. – Let $p,q,r \in N_0$ and $n_3,n_4 \in N$ such that $p+q+r = n_3+n_4$. If

$$\left[\begin{matrix}(p \leq n_3)\ \text{and}\ (r \leq n_4)\ \text{and}\ (p+r \leq n_3+n_4-1)\\ \text{and}\ (q \leq 3n_3 - 2p)\ \text{and}\ (q \leq 4n_4 - 2r)\end{matrix}\right],$$

then F $(n_3, n_4, p, q, r) \neq \varnothing$.

Proof. Let us describe a graph $G \in$ F (n_3, n_4, p, q, r). If $n_3 = 1$ and $p = 0$, then $G[N_3]$ is a graph with no edges; if $n_3 = 1$ and $p = 1$ then $G[N_3]$ is a graph with a single vertex and a loop; if $n_3 = p$ and $n_3 = 2$, then $G[N_3]$ is a graph with two vertices and two parallel edges adjacent to them; if $n_3 = p$ and $n_3 > 2$, then $G[N_3]$ is a cycle; if $n_3 \geq 2$ and $p \leq \frac{n_3}{2}$, then $G[N_3]$ is a graph such that $\Delta(G(N_3)) \leq 1$; if $n_3 \geq 2$ and $\frac{n_3}{2} < p \leq n_3 - 1$, then $G[N_3]$ is an acyclic graph such that $\delta(G(N_3)) \geq 1$ and that $\Delta(G(N_3)) \leq 2$.

If $n_4 = 1$ and $r = 0$, then $G[N_4]$ is a graph with no edges; if $n_4 = 1$ and $r = 1$, then $G[N_4]$ is a graph with a single vertex and a loop; if $n_4 = r$ and $n_4 = 2$, then $G[N_4]$ is a graph with two vertices and two parallel edges adjacent to them; if $n_4 = r$ and $n_4 > 2$, then $G[N_4]$ is a cycle; if $n_4 \geq 2$ and $r \leq \frac{n_4}{2}$, then $G[N_4]$ is a graph such that $\Delta(G(N_4)) \leq 1$;

if $n_4 \geq 2$ and $\frac{n_4}{2} < r \leq n_4 - 1$, then $G[N_4]$ is an acyclic graph such that $\delta(G(N_4)) \geq 1$ and that $\Delta(G(N_4)) \leq 2$.

We distinguish three cases:

1) $(n_3 = 1)$ and $(p = 0)$ and $(r = 0)$.

Note that $q = n_3 + n_4 - p - r = n_4 + 1 \leq 3n_3 - 2p = 3$, hence $1 \leq n_4 \leq 2$. If $n_4 = 1$, then G is the graph with two vertices adjacent with two parallel edges; and if $n_4 = 2$, then G is the graph such that $V(G) = \{x_1, y_1, y_2\}$ and $E(G) = \{x_1y_1, x_1y_1, x_1y_2\}$.

2) $(n_4 = 1)$ and $(p = 0)$ and $(r = 0)$.

This case can be solved analogously as the previous one.

3) $[(n_3 > 1)$ and $(n_4 > 1)]$ or $(p > 0)$ or $(r > 0)$.

Note that $\max\{4 - d_G(y_1),\ldots, 3 - d_G(y_{n_4})\} - \min\{4 - d_G(y_1),\ldots, 4 - d_G(y_{n_4})\} \leq 1$. So, from the previous Lemma, it follows that it is sufficient to prove that

$$q \leq \min\left\{\sum_{i=1}^{n_3}\min\{3-d_G(x_i),n_4\},\sum_{i=1}^{n_4}\left(4-d_G(y_i)\right)\right\}.$$

Note, that $\max\{3 - d_G(x_1),\ldots, 3 - d_G(x_{n_3})\} - \min\{3 - d_G(x_1),\ldots, 3 - d_G(x_{n_3})\} \leq 1$. Therefore, the above expression is equivalent to

$$q \leq \min\left\{\sum_{i=1}^{n_3}\min\{3-d_G(x_i)\},\sum_{i=1}^{n_4}\left(4-d_G(y_i)\right),n_3n_4\right\}.$$

Simple computation shows that this is equivalent to

$$q \leq \min\{3n_3 - 2m_{33}, 4n_4 - 2m_{44}, n_3n_4\}.$$

It remains to prove that $q \leq n_3n_4$. Distinguish three subcases:

3.1) $(p > 0)$ or $(r > 0)$.

Note that $(n_3 - 1)(n_4 - 1) \geq 0$, hence $q = n_3 + n_4 - p - q - r \leq n_3 + n_4 - 1 \leq n_3n_4$.

3.2) $(n_3 > 1)$ and $(n_4 > 1)$.

Suppose to the contrary that $q > n_3n_4$. Note that $q = n_3 + n_4 - p - r \leq n_3 + n_4$. It follows that $n_3n_4 < n_3 + n_4$. Now, we have $2n_3 < n_3n_4 < n_3 + n_4$ and $2n_4 < n_3n_4 < n_3 + n_4$, which implies $n_3 < n_4$ and $n_4 < n_3$, which is a contradiction.

Lemma 4. – Let $p,q,r \in N_0$ and $n_3,n_4 \in N$ such that $p + q + r = n_3 + n_4$. If

$$\begin{bmatrix}(p \leq n_3) \text{ and } (r \leq n_4) \text{ and } (p+r \leq n_3+n_4-1) \\ \text{and } (q \leq 3n_3-2p) \text{ and } (q \leq 4n_4-2r)\end{bmatrix},$$

then there is at least one connected graph in F (n_3, n_4, p, q, r).

Proof. Let G' be a graph constructed in the previous Lemma. Let $\mathring{G}$ be a set of graphs G'' $\in$ F (n_3, n_4, p, q, r) and such that $G''[N_3] = G'[N_3]$ and $G''[N_4] = G'[N_4]$. Note that $\mathring{G}$ is nonempty, since at least G' is in $\mathring{G}$. Let G be a graph in $\mathring{G}$ with the smallest number of connected components. It remains to prove that G is connected. Suppose the contrary. Then, there is at least one component C (in G) and an edge e such that:

a) e is not one of parallel edges;
b) $e \in E_G(N_3, N_4)$;
c) e is contained in a cycle.

Denote $e = xy$, such that $x \in N_3$ and $y \in N_4$. Let C' be any other component. Distinguish three cases:

1) $V(C') \subseteq N_3$.

Let $c \in V(C')$ be an arbitrary vertex. Graph $G - xy + yc$ is in $\mathring{G}$ and it has a smaller number of components than G, which is a contradiction.

2) $V(C') \subseteq N_4$.

Let $c \in V(C')$ be an arbitrary vertex. Graph $G - xy + xc$ is in $\mathring{G}$ and it has a smaller number of components than G, which is a contradiction.

3) $V(C') \cap N_3 \neq \emptyset$ and $V(C') \cap N_4 \neq \emptyset$.

There is an edge $x'y'$ such that $x' \in N_3$ and $y' \in N_4$ in C'. Graph $G - xy + x'y' + xy' + x'y$ is in $\mathring{G}$ and it has a smaller number of components then G, what is a contradiction.

We have obtained a contradiction in each case, so our claim is proved.

Now, we shall prove four theorems that cover four different cases:

1) $m_{13} + m_{23} + m_{33} + m_{34} > 0$ and $m_{14} + m_{24} + m_{34} + m_{44} > 0$;
2) $m_{13} + m_{23} + m_{33} + m_{34} = 0$ and $m_{14} + m_{24} + m_{34} + m_{44} > 0$;
3) $m_{13} + m_{23} + m_{33} + m_{34} > 0$ and $m_{14} + m_{24} + m_{34} + m_{44} = 0$;
4) $m_{13} + m_{23} + m_{33} + m_{34} = 0$ and $m_{14} + m_{24} + m_{34} + m_{44} = 0$.

Theorem 5. **–** Let $m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in \mathcal{N}$ such that $m_{13} + m_{23} + m_{33} + m_{34} > 0$ and that $m_{14} + m_{24} + m_{34} + m_{44} > 0$. There is a molecular graph G such that $\mu(G) = m$ if and only if the following holds:

$$\left[\begin{array}{l} (m_{11}=0) \text{ and } [(m_{12}+m_{23}+m_{24}>0) \text{ or } \\ (m_{22}=0)] \text{ and } (n_2, n_3, n_4 \in N_0) \text{ and } (x \geq 0) \\ \text{and } (m_{33} \leq n_3) \text{ and } (m_{33}+x-m_{24} \leq n_3) \text{ and } \\ (m_{44} \leq n_4) \text{ and } (m_{44}+x-m_{23} \leq n_4) \\ \text{and } (m_{33}+m_{34}+m_{44}+x = n_3+n_4) \text{ and } \\ (m_{33}+m_{44} \leq n_3+n_4-1) \\ \text{and } (m_{33}+m_{44}+x-m_{23} \leq n_3+n_4-1) \text{ and } \\ (m_{33}+m_{44}+x-m_{24} \leq n_3+n_4-1) \\ \text{and } ((n_3>1) \text{ or } ((m_{34} \leq n_4) \text{ and } (m_{33}=0))) \\ \text{and } ((n_4>1) \text{ or } ((m_{34} \leq n_3) \text{ and } (m_{44}=0))) \\ \text{and } ((n_3>2) \text{ or } (m_{33}<n_3)) \text{ and } ((n_4>2) \text{ or } \\ (m_{44}<n_4)) \\ \text{and } ((n_3>1) \text{ or } (x-m_{24} \leq 0) \text{ or } (m_{22} \geq 1)) \text{ and } \\ ((n_4>1) \text{ or } (x-m_{23} \leq 0) \text{ or } (m_{22} \geq 1)) \\ \text{and } ((n_3>1) \text{ or } (n_4>1) \text{ or } (x-m_{23} \leq 0) \text{ or } \\ (x-m_{24} \leq 0) \text{ or } (m_{22} \geq 2)) \end{array}\right],$$

where

$$n_2 = (m_{12} + 2m_{22} + m_{23} + m_{24})/2$$

$$n_3 = (m_{13} + m_{23} + 2m_{33} + m_{34})/3$$

$$n_4 = (m_{14} + m_{24} + m_{34} + 2m_{44})/4$$

$$x = (m_{23} + m_{24} - m_{12})/2.$$

Proof. Let us first prove the necessity. We shall define graph G with the required properties. Note that: $m_{12} + 2m_{22} + m_{23} + m_{24} \equiv m_{23} + m_{24} - m_{12} \pmod 2$, therefore $x \in N_0$. By a tedious check of twelve inequalities, it can be proved that

$$\max\{x - m_{24}, 0\} \leq$$

$$\min\left\{\begin{array}{l} x,\ n_3+n_4-m_{33}-m_{44}-1,\ \dfrac{m_{23}}{2},\ n_4-m_{44}-x+m_{23}, \\ \dfrac{n_3+n_4-1-m_{33}-m_{44}-x+m_{23}}{2},\ n_3-m_{33} \end{array}\right\}.$$

Hence, by putting $p' = \max\{x - m_{24}, 0\} \in N_0$, we get

$$\max\{x - m_{24}, 0\} \leq p' \leq$$

$$\min.\left\{\begin{array}{l} x, n_3+n_4-m_{33}-m_{44}-1, \dfrac{m_{23}}{2}, n_4-m_{44}-x+m_{23}, \\ \dfrac{n_3+n_4-1-m_{33}-m_{44}-x+m_{23}}{2},\ n_3-m_{33} \end{array}\right\}.$$

Again, by a tedious check of eight inequalities, it can be proved that

$$\max\{0, p' + x - m_{23}\} \leq \min\{x - p', p' - x + m_{24}, n_4 - m_{44}, n_3 + n_4 - 1 - m_{33} - m_{44} - p'\}.$$

Therefore, by putting $r' = \max\{0, p' + x - m_{23}\} \in \boldsymbol{N}_0$, we get

$$\max\{0, p' + x - m_{23}\} \leq r' \leq \min\{x - p', p' - x + m_{24}, n_4 - m_{44}, n_3 + n_4 - 1 - m_{33} - m_{44} - p'\}.$$

Since $x \geq p' + r'$, it follows that $q' = x - p' - r' \in \boldsymbol{N}_0$. Denote $p = m_{33} + p'$, $q = m_{34} + q'$, and $r = m_{44} + r'$. Note that

$$\left[\begin{array}{l} (p \leq n_3) \text{ and } (r \leq n_4) \text{ and } (p+r \leq n_3+n_4-1) \\ \text{and } (q \leq 3n_3-2p) \text{ and } (q \leq 4n_4-2r) \end{array}\right],$$

hence there is a connected graph $G' \in F(n_3, n_4, p, q, r)$ constructed in the previous lemma. Let us select p' edges in $E_{G'}(N_3)$, q' edges in $E_{G'}(N_3, N_4)$ and r' edges in $E_{G'}(N_4)$ such that the remaining graph is simple. Note that this is always possible, because

$$\left[\begin{array}{l} (m_{33} \leq n_3) \text{ and } (m_{44} \leq n_4) \text{ and } \\ (m_{33}+m_{34}+m_{44} \leq n_3+n_4) \\ \text{and } (m_{33}+m_{44} \leq n_3+n_4-1) \text{ and } ((n_3>1) \text{ or } \\ ((m_{34} \leq n_4) \text{ and } (m_{33}=0))) \\ \text{and } (2m_{33}+m_{34} \leq n_3) \text{ and } (2m_{34}+m_{34} \leq n_4) \\ \text{and } ((n_3>1) \text{ or } ((m_{34} \leq n_4) \text{ and } (m_{33}=0))) \\ \text{and } ((n_4>1) \text{ or } ((m_{34} \leq n_4) \text{ and } (m_{44}=0))) \\ \text{and } ((n_3>2) \text{ or } (m_{33}<n_3)) \text{ and } ((n_4>2) \text{ or } \\ (m_{44}<n_4)) \\ \text{and } (2m_{33}+m_{34} \leq n_3) \text{ and } (2m_{34}+m_{34} \leq n_4) \end{array}\right].$$

Let G'' be a graph obtained by replacing each of the selected edges by a path of length 2, by adding to each vertex x in N_3 exactly $3 - d_{G'}(x)$ neighbors of degree 1, and by adding to each y vertex in N_4 exactly $4 - d_{G'}(y)$ neighbors of degree 1. Note that: $3n_3 - 2p - q \geq m_{23} - 2p' - q' \geq 0$ and that: $4n_4 - 2r - q \geq m_{24} - 2r' - q' \geq 0$, therefore it is possible to select $m_{23} - 2p' - q'$ edges that connect vertices of degrees 1 and 3; and to select $m_{24} - 2q' - r'$ edges that connect vertices of degrees 1 and 3. Let G''' be a graph obtained by replacing each of these vertices by a path of length 2. Note that:

$$\mu(G''') = (m_{11}, m_{12}, m_{13}, m_{14}, 0, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$$

Distinguish three cases:

1) G''' is a simple graph.

If $m_{22} = 0$, it is sufficient to take G = G'''. Otherwise, denote by z an arbitrary vertex of degree 2 and denote neighbors of z by z' and z''. Graph G is defined by

$$V(\mathrm{G}) = V(\mathrm{G}''') \cup \{z_0, z_1,\ldots, z_{m_{22}}\} \setminus \{z\}$$

$$E(\mathrm{G}) = E(\mathrm{G}''') \cup \{z'z_0, z_0z_1, z_1z_2,\ldots, z_{m_{22}-1}z_{m_{22}}, z_{m_{22}}z''\} \setminus \{z'z, z''z\}$$

2) G''' contains no loops and a single pair of parallel edges.

We have one of the following two subcases:

2.1) ($n_3 = 1$) and ($x - m_{24} > 0$), and vertices adjacent to parallel edges have degrees 2 and 3.

2.2) ($n_4 = 1$) and ($x - m_{23} > 0$), and vertices adjacent to parallel edges have degrees 2 and 4.

In both of these subcases denote by z a vertex of degree 2 adjacent to these parallel edges and by z' another vertex adjacent to these edges. Graph G is defined by

$$V(\mathrm{G}) = V(\mathrm{G}''') \cup \{z_0, z_1,\ldots, z_{m_{22}}\} \setminus \{z\}$$

$$E(\mathrm{G}) = E(\mathrm{G}''') \cup \{z'z_0, z_0z_1, z_1z_2,\ldots, z_{m_{22}-1}z_{m_{22}}, z_{m_{22}}z'\} \setminus \{z'z, z'z\}.$$

3) G''' contains no loops and it has two pairs of parallel edges.

We have ($n_3 = 1$) and ($n_4 = 1$) and ($x - m_{23} > 0$) and ($x - m_{24} > 0$). One pair of parallel edges is adjacent to vertices of degree 2 (denote it by z) and 3 (denote it by z') and the other is adjacent to vertices of degree 2 (denote it by w) and 4 (denote it by w'). Note that, in this case, $m_{22} \geq 2$. Graph G is defined by

$$V(\mathrm{G}) = V(\mathrm{G}''') \cup \{w_0, w_1\} \cup \{z_0, z_1,\ldots, z_{m_{22}-1}\} \setminus \{z,w\}$$

$$E(\mathrm{G}) = E(\mathrm{G}''') \cup \{z'z_0, z_0z_1, z_1z_2,\ldots, z_{m_{22}-2}z_{m_{22}-1}z', w'w_0, w_0w_1\ w_1w'\} \setminus \{z'z, z'z, w'w, w'w\}$$

All the cases are exhausted and the necessity is proved.

Now, let us prove sufficiency. Let G be a graph with the required properties. Note that G has n_j vertices of degree j, for each $j = 2,3,4$, so indeed $n_2, n_3, n_4 \in N_0$. Since G is connected and $n_3, n_4 > 0$, it follows that [($m_{12} + m_{23} + m_{24} > 0$) or ($m_{22} = 0$)] and that $m_{11} = 0$. Since G is simple, it follows that (($n_3 > 1$) or (($m_{34} \leq n_3$) and ($m_{33} = 0$))); and that (($n_4 > 1$) or (($m_{34} \leq n_4$) and ($m_{44} = 0$))); and that (($n_3 > 2$) or ($m_{33} < n_3$)) and (($n_4 > 2$) or ($m_{44} < n_4$)). Denote by N_i the set of vertices of degree i (in G) for each $i = 2,3,4$. Note that G[N_3] and G[N_4] have at most one cycle and not both of them contain a cycle. Hence, $m_{33} \leq n_3$, $m_{44} \leq n_4$ and $m_{33} + m_{44} \leq n_3 + n_4 - 1$. Denote by P the set of all maximal induced paths in G such that its all interior vertices have degree 2 (in G). Denote by P_{ij}, $i \leq j$ the set of paths in P such that its terminal vertices have degrees i and j. Note that P is partitioned in the sets P_{13}, P_{14}, P_{33}, P_{34} and P_{44}. Denote $P' = P_{33} \cup P_{34} \cup P_{44}$. Note that there are exactly x paths in P', so indeed $x \geq 0$. Let G' be a graph obtained by a contraction of all paths in P' to a single edge. Graph G'[$N_3 \cup N_4$] is a monocyclic graph, therefore $m_{33} + m_{34} + m_{44} + x = n_3 + n_4$. Note that G'[$N_3$] and G'[$N_4$] have at most one cycle and not both of them contain a cycle, therefore

$$n_3 + n_4 \geq m_{33} + |P_{33}| + m_{44} - 1 \geq m_{33} + m_{44} + (x - m_{24}) - 1$$

$$n_3 + n_4 \geq m_{33} + |P_{44}| + m_{44} - 1 \geq m_{33} + m_{44} + (x - m_{23}) - 1$$

Let G'' be a graph obtained by a contraction of all paths in P_{33} to a single edge. Since G''[N_3] has at most one cycle, it follows that $n_3 \geq m_{33} + |P_{33}| \geq m_{33} + (x - m_{24})$. Also if $n_3 = 1$ and $m_{22} = 0$, then $0 = |P_{33}| \geq x - m_{24}$, hence ($n_3 > 1$) or ($x - m_{24} \leq 0$) or ($m_{22} \geq 1$).

Analogously, let G''' be a graph obtained by a contraction of all paths in P_{44} to a single edge. Since G'''[N_4] has at most one cycle, it follows that $n_4 \geq m_{44} + |P_{44}| \geq m_{44} + (x - m_{23})$. Also, if $n_4 = 1$ and $m_{22} = 0$, then $0 = |P_{44}| \geq x - m_{23}$, hence ($n_4 > 1$) or ($x - m_{23} \leq 0$) or ($m_{22} \geq 1$).

Analogously, it can be proved that

$$(n_3 > 1) \text{ or } (n_4 > 1)\ (x - m_{23} \leq 0) \text{ or } (x - m_{24} \leq 0) \text{ or } (m_{22} \geq 2).$$

This proves the theorem.

Let us prove:

Theorem 6. – Let $m = (m_{11}, m_{12}, 0, m_{14}, m_{22}, 0, m_{24}, 0, 0, m_{44}) \in \mathbb{N}_0^{10}$ such that $m_{14} + m_{24} + m_{44} > 0$. There is a monocyclic molecular graph G such that $\mu(\mathrm{G}) = m$ if and only if

$$\left[\begin{array}{l} (m_{11}=0) \text{ and } ((m_{22}=0) \text{ or } (m_{12}+m_{24}>0)) \text{ and } (n_2, n_4) \in \mathbb{N}_0) \\ \text{and } (x \geq 0) \text{ and } (m_{44}+x=n_4) \text{ and } ((n_4 \neq 2) \text{ or } (m_{44}<2)) \\ \text{and } ((n_4 \neq 1) \text{ or } ((m_{22}>0) \text{ and } (m_{44}=0))) \end{array}\right]$$

where

$$n_2 = (m_{12} + 2m_{22} + m_{24})/2$$

$$n_4 = (m_{14} + m_{24} + 2m_{44})/4$$

$$x = (m_{24} - m_{12})/2.$$

Proof. First let us prove the necessity. We shall define graph G with the required properties. Note that $m_{12} + 2m_{22} + m_{24} \equiv m_{24} - m_{12} \pmod 2$, hence $x \in \mathcal{N}_0$. Distinguish three cases:

1) $n_4 = 1$.

Let G' be the graph defined by

$$V(G) = \{a, b_0, b_1, \ldots, b_{m_{22}}, c_1, c_2\}$$

$$E(G) = \{ab_0, b_0b_1, b_1b_2, \ldots, b_{m_{22}-1}b_{m_{22}}, bm_{22}a, ac_1, ac_2\}$$

Graph G is obtained from G' by replacing arbitrary m_{12} edges from the set $\{ac_1, ac_2\}$ by paths of length 2.

2) $n_4 = 2$.

We start from graph G' defined by

$$V(\mathrm{G}') = \begin{cases} \{a_1, a_2, b_1, c_1, c_2, c_3, c_4\}, m_{44} = 1 \\ \{a_1, a_2, b_1, b_2, c_1, c_2, c_3, c_4\}, m_{44} = 0 \end{cases}$$

$E(\mathrm{G}') =$

$$\begin{cases} \{a_1a_2, a_1b_1, a_2b_1, a_1c_1, a_1c_2, a_2c_3, a_2c_4\}, m_{44}=1 \\ \{a_1b_1, a_2b_1, a_1b_2, a_2b_2, a_1c_1, a_1c_2, a_2c_3, a_2c_4\}, m_{44}=0. \end{cases}$$

Let graph G'' be obtained from G' by replacing arbitrary m_{12} edges from the set $\{a_1c_1, a_1c_2, a_2c_3, a_2c_4\}$ by paths of length 2. If $m_{22} = 0$, it is sufficient to take G = G''. Otherwise, define G by:

$$V(\mathrm{G}) = V(\mathrm{G}'') \cup \{d_0, d_1, \ldots, d_{m_{22}}\} \setminus \{b_1\}$$

$$E(\mathrm{G}) = E(\mathrm{G}'') \cup \{a_1d_0, d_0d_1, d_1d_2, \ldots, d_{m_{22}-1}d_{m_{22}}, d_{m_{22}}a_2\} \setminus \{a_1b, ba_2\}.$$

3) $n_4 \geq 3$.

Let G' be a cycle with n_4 vertices. Let G'' be a graph obtained by replacing arbitrary x edges by paths of length 2 and adding to each vertex in G' two neighbors of degree 1. Let G''' be a graph obtained from G'' by replacing arbitrary x edges adjacent to vertices of degree 1 by paths of length 2. Note that $\mu(\mathrm{G}''') = (m_{11}, m_{12}, 0, m_{14}, 0, 0, m_{24}, 0, 0, m_{44})$. If $m_{22} = 0$, it is sufficient to take G = G'''. Otherwise, let z be a vertex of degree 2 in G''' and let z' and z'' be its neighbors. Graph G is defined by

$$V(\mathrm{G}) = V(\mathrm{G}''') \cup \{z_0, z_1, \ldots, z_{m_{22}}\} \setminus \{z\}$$

$$E(\mathrm{G}) = E(\mathrm{G}''') \cup \{ z'z_0, z_0z_1, z_1z_2, \ldots, z_{m_{22}-1}z_{m_{22}}, z_{m_{22}}z'\} \setminus \{zz', zz''\}.$$

All the cases are exhausted and the necessity is proved.

Now, let us prove sufficiency. Let G be the graph with the required properties. Denote N_2, N_4, n_2, n_4, P, P_{14} and P_{44} as in the previous theorem. Obviously, $n_2, n_4 \in \mathcal{N}_0$ and since G is connected, it directly follows that ($m_{11} = 0$) and (($m_{22} = 0$) or ($m_{12} + m_{24} > 0$)). Note that $x = |P_{44}|$, hence ($x \geq 0$) and ($m_{44} + x = n_4$). If $n_4 = 2$, then $m_{44} < 2$. Therefore, we have ($n_4 \neq 2$) or ($m_{44} < 2$). Also, if $n_4 = 1$, then $m_{22} > 0$ and $m_{44} = 0$, hence indeed

$$(n_4 \neq 1) \text{ or } ((m_{22} > 0) \text{ and } (m_{44} = 0)).$$

This proves the theorem.

By a complete analogy, it can be proved that:

Theorem 7. – Let $m = (m_{11}, m_{12}, m_{13}, 0, m_{22}, m_{23}, 0, m_{33}, 0, 0) \in N_0^{10}$ such that $m_{13} + m_{23} + m_{33} > 0$. There is a monocyclic molecular graph G such that $\mu(\mathrm{G}) = m$ if and only if

$$\begin{bmatrix} (m_{11} = 0) \text{ and } ((m_{22} = 0) \text{ or } (m_{12} + m_{23} > 0)) \text{ and } \\ (n_2, n_3 \in \mathcal{N}_0) \\ \text{and } (x \geq 0) \text{ and } (m_{33} + x = n_3) \text{ and } ((n_3 \neq 2) \text{ or } \\ (m_{33} < 2)) \\ \text{and } ((n_3 \neq 1) \text{ or } ((m_{22} > 0) \text{ and } (m_{33} = 0))) \end{bmatrix}$$

where

$$n_2 = (m_{12} + 2m_{22} + m_{23})/2$$

$$n_3 = (m_{13} + m_{23} + 2m_{33})/3$$

$$x = (m_{23} - m_{12})/2.$$

It can be easily proved that:

Theorem 8. – Let $m = (m_{11}, m_{12}, 0, 0, m_{22}, 0, 0, 0, 0, 0) \in N_0^{10}$. There is a monocyclic molecular graph G such that $\mu(\mathrm{G}) = m$ if and only if [($m_{11} = 0$) and ($m_{12} = 0$) and ($m_{22} \geq 3$].

ALGORITHM

In this section, we present the main result of our paper. We present an algorithm that generates the set $\mu(A_n)$. We use Theorem 5 to make function gen1; we use Theorem 6 to make function gen2; Theorem 7 is used to make function gen3; and Theorem 8 is incorporated within the code of the function gen. The code is presented in the programming language C++. The function xx is any user defined function that utilizes this algorithm.

```
void gen1 ( int n )
{ int n1, n2, n3, n4, m12, m13, m14, m22, m23, m24, m33, m34, m44, x;
  if ( 5 <= n )
  {for ( n4 = 1; n4 <= (n - 2) / 3; n4++ )
    for ( n3 = 1; 3 * n4 + 2 * n3 <= n; n3++ )
    {n1 = 2 * n4 + n3;
     n2 = n - n1 - n3 - n4;
     for ( m12 = 0; m12 <= min ( n1, 2 * n2 ); m12++ )
       for ( m13= 0; m13 <= min ( n1 - m12, 3 * n3 ); m13++ )
       {m14 = n1 - m12 - m13;
        if ( m14 + 1 <= 4 * n4 )
         {for ( m22 = 0; m12 + 2 * m22 <= 2 * n2; m22++ )
           for ( m23 = 0; m23 <= min (2 * n2 - m12 - 2 * m22, 3 * n3 - m13 ); m23++ )
           {m24 = 2 * n2 - m12 - 2 * m22 - m23;
             if ( m14 + m24 <= 4 * n4 )
              for ( m33 = 0; m33 <= min ( (3 * n3 - m13 - m23) / 2, n3); m33++)
              {m34 = 3 * n3 - m13 - m23 - 2 * m33;
                m44 = ( 4 * n4 - m14 - m24 - m34 ) / 2;
                x = (m24 + m23 - m12) / 2;
                if ( (x >= 0) && (m44 <= n4) && (0 <= m44) &&
                       (x - m24 + m33 <= n3) && (x - m23 + m44 <= n4) &&
                       ( (m22 == 0) || (m12 + m23 + m24 > 0) ) &&
                       ( m33 + m34 + m44 + x == n3 + n4 ) &&
                       ( m33 + m44 <= n3 + n4 - 1 ) &&
                       ( m33 + m44 + x - m23 <= n3 + n4 - 1 ) &&
                       ( m33 + m44 + x - m24 <= n3 + n4 - 1 ) &&
                       ( (n3 > 1) || ((m34 <= n4) && (m33 == 0)) ) &&
                       ( (n4 > 1) || ((m34 <= n3) && (m44 == 0)) ) &&
                       ( (n3 > 2) || (m33 < n3) ) &&
                       ( (n4 > 2) || (m44 < n4) ) &&
                       ( (n3 > 1) || (x - m24 <= 0) || (m22 >= 1) ) &&
                       ( (n4 > 1) || (x - m23 <= 0) || (m22 >= 1) ) &&
                       ( (n4 > 1) || (n3 > 1) || (x - m23 <= 0) ||
                          (x - m24 <= 0) || (m22 >= 1)
                       )
                    )
                 xx ( 0, m12, m13, m14, m22, m23, m24, m33, m34, m44 );
              }
           }
         }
       }
    }
  }
}
//---------------------------------------------------------------
void gen2 ( int n )
{ int n1, n2, n4, m12, m14, m22, m24, m44, x;
  if ( 1 <= n / 3 )
   for ( n4 = 1; n4 <= n / 3; n4++ )
    { n1 = 2 * n4;
      n2 = n - n1 - n4;
      for ( m12 = 0; m12 <= min ( n1, n2 ); m12++ )
      { m14 = n1 - m12;
        if ( m14 <= 4 * n4 - 1 )
          for ( m44 = 0; 2 * m44 <= 4 * n4 - m14; m44++ )
          { m24 = 4 * n4 - 2 * m44 - m14;
            if ( (m24 >= m12) && ( (m24 + m12) % 2) == 0 && (2 * n2 >= m24 + m12) )
            { x = (m24 - m12) / 2;
              m22 = (2 * n2 - m12 - m24) / 2;
              if ( ((m22 == 0) || (m12 + m24 > 0))  && (m44 + x == n4) &&
                     ((n4 != 2) || (m44 < 2)) &&
                     ( (n4 != 1) || ((m22 > 0) && (m44 == 0)) )
                 )
                  xx ( 0, m12, 0, m14, m22, 0, m24, 0, 0, m44 );
            }
          }
      }
    }
}
//---------------------------------------------------------------
void gen3 ( int n )
{ int n1, n2, n3, m12, m13, m22, m23, m33, x;
  if ( 2 <= n )
   for ( n3 = 1; n3 <= n / 2; n3++ )
    { n1 = n3;
      n2 = n - n1 - n3;
      for ( m12 = 0; m12 <= min ( n1, n2 ); m12++ )
      { m13 = n1 - m12;
        if ( m13 <= 3 * n3 - 1 )
          for ( m33 = 0; 2 * m33 <= 3 * n3 - m13; m33++ )
          { m23 = 3 * n3 - 2 * m33 - m13;
            if ( (m23 >= m12) && ( (m23 + m12) % 2) == 0 && (2 * n2 >= m23 + m12) )
            { x = (m23 - m12) / 2;
              m22 = (2 * n2 - m12 - m23) / 2;
              if ( ((m22 == 0) || (m12 + m23 > 0))  && (m33 + x == n3) &&
                     ((n3 != 2) || (m33 < 2)) &&
                     ( (n3 != 1) || ((m22 > 0) && (m33 == 0)) )
                 )
                  xx ( 0, m12, m13, 0, m22, m23, 0, m33, 0, 0 );
            }
          }
      }
    }
}
//---------------------------------------------------------------
void gen ( int n )
{ gen1 ( n );
  gen2 ( n );
  gen3 ( n );
  if ( n >= 3 )
    xx ( 0, 0, 0, 0, n, 0, 0, 0, 0, 0 );
}
```

DISCRIMINATIVE PROPERTIES OF THE ZAGREB AND MODIFIED ZAGREB INDICES FOR MONOCYCLIC GRAPHS

The aim of this section is to utilize the developed algorithm. We compare discriminative properties of the Zagreb, M_2, and modified Zagreb, $^*M_2$, indices for monocyclic graphs with the prescribed number of vertices,

Let n be a natural number larger than 5. Define the following functions $(M_2)_n$, $(^*M_2)_n : \mu(A_n) \rightarrow R$, which map 10-tuples into real numbers by

$$(M_2)_n\ (\mu(\mathrm{G})) = M_2(\mathrm{G})$$

$$(^*M_2)_n\ (\mu(\mathrm{G})) = {}^*M_2(\mathrm{G})$$

We also define

$$P_n = \{\{m_1, m_2\}: m_1, m_2 \in \mu(A_n), m_1 \neq m_2\}$$

$$D_n = \{\{m_1, m_2\} \in P_n : m_1, m_2 \in \mu(A_n), (M_2)_n\ (m_1) \neq (M_2)_n\ (m_2)\}$$

$$^*D_n = \{\{m_1, m_2\} \in P_n : m_1, m_2 \in \mu(A_n), (^*M_2)_n\ (m_1) \neq (^*M_2)_n\ (m_2)\}$$

$$I_n = \{\{m_1, m_2\} \in P_n : m_1, m_2 \in \mu(A_n), (M_2)_n\ (m_1) = (M_2)_n\ (m_2)\}$$

$$^*I_n = \{\{m_1, m_2\} \in P_n : m_1, m_2 \in \mu(A_n), (^*M_2)_n\ (m_1) = (^*M_2)_n\ (m_2)\}$$

The probability that the pair of elements of $\mu(A_n)$ will be discriminated by the Zagreb indices is $|D_n|/|P_n|$ and probability that they will not be discriminated is $|I_n|/|P_n|$. Analogously, the probability that the pair of elements of $\mu(A_n)$ will be discriminated by modified Zagreb indices is $|D^*_n|/|P_n|$ and probability that they will not be discriminated is $|I^*_n|/|P_n|$. Computations for graphs containing up to $n = 60$ vertices are given (right column).

These results show that both the Zagreb and modified Zagreb indices have remarkable discriminative properties with relative discrimination monotonously increasing with n for both indices. (Note that here discrimination refers to the allowed 10-tuples rather than to the corresponding graph(s).)

n	$\|I_n\|/\|P_n\|$	$\|D_n\|/\|P_n\|$	$\|^*I_n\|/\|P_n\|$	$\|^*D_n\|/\|P_n\|$	$\|^*I_n\|/\|I_n\|$
5	0.00000000	1.00000000	0.10000000	0.90000000	Not defined
6	0.02222222	0.97777778	0.04444444	0.95555556	2.00000000
7	0.02857143	0.97142857	0.04285714	0.95714286	1.50000000
8	0.04390244	0.95609756	0.03902439	0.96097561	0.88888889
9	0.03725222	0.96274778	0.02836637	0.97163363	0.76146789
10	0.03954248	0.96045752	0.02407407	0.97592593	0.60881543
11	0.03762765	0.96237235	0.02060826	0.97939174	0.54768928
12	0.03696362	0.96303638	0.01793501	0.98206499	0.48520710
13	0.03513187	0.96486813	0.01555096	0.98444904	0.44264549
14	0.03381267	0.96618733	0.01374751	0.98625249	0.40657877
15	0.03207130	0.96792870	0.01239674	0.98760326	0.38653691
16	0.03077980	0.96922020	0.01128480	0.98871520	0.36663021
17	0.02941603	0.97058397	0.01029388	0.98970612	0.34994106
18	0.02829158	0.97170842	0.00949273	0.99050727	0.33553192
19	0.02717207	0.97282793	0.00883651	0.99116349	0.32520573
20	0.02620563	0.97379437	0.00826711	0.99173289	0.31547076
21	0.02527772	0.97472228	0.00777711	0.99222289	0.30766641
22	0.02446684	0.97553316	0.00735401	0.99264599	0.30057051
23	0.02366843	0.97633157	0.00696909	0.99303091	0.29444672
24	0.02296025	0.97703975	0.00663049	0.99336951	0.28878139
25	0.02226977	0.97773023	0.00632713	0.99367287	0.28411294
26	0.02162345	0.97837655	0.00605249	0.99394751	0.27990382
27	0.02100165	0.97899835	0.00580188	0.99419812	0.27625816
28	0.02041697	0.97958303	0.00557380	0.99442620	0.27299854
29	0.01984925	0.98015075	0.00536252	0.99463748	0.27016263
30	0.01931456	0.98068544	0.00516939	0.99483061	0.26764210
31	0.01879824	0.98120176	0.00499049	0.99500951	0.26547634
32	0.01830773	0.98169227	0.00482385	0.99517615	0.26348684
33	0.01783646	0.98216354	0.00466854	0.99533146	0.26174122
34	0.01738830	0.98261170	0.00452391	0.99547609	0.26016976
35	0.01695699	0.98304301	0.00438799	0.99561201	0.25877184
36	0.01654679	0.98345321	0.00426082	0.99573918	0.25750160
37	0.01615197	0.98384803	0.00414115	0.99585885	0.25638655
38	0.01577537	0.98422463	0.00402826	0.99597174	0.25535145
39	0.01541336	0.98458664	0.00392158	0.99607842	0.25442727
40	0.01506812	0.98493188	0.00382085	0.99617915	0.25357206
41	0.01473576	0.98526424	0.00372521	0.99627479	0.25280048
42	0.01441821	0.98558179	0.00363458	0.99636542	0.25208266
43	0.01411266	0.98588734	0.00354843	0.99645157	0.25143623
44	0.01382003	0.98617997	0.00346640	0.99653360	0.25082409
45	0.01353828	0.98646172	0.00338819	0.99661181	0.25026721
46	0.01326825	0.98673175	0.00331364	0.99668636	0.24974196
47	0.01300792	0.98699208	0.00324232	0.99675768	0.24925759
48	0.01275801	0.98724199	0.00317420	0.99682580	0.24880024
49	0.01251696	0.98748304	0.00310895	0.99689105	0.24837929
50	0.01228519	0.98771481	0.00304642	0.99695358	0.24797473
51	0.01206143	0.98793857	0.00298642	0.99701358	0.24760086
52	0.01184603	0.98815397	0.00292884	0.99707116	0.24724247
53	0.01163783	0.98836217	0.00287346	0.99712654	0.24690727
54	0.01143715	0.98856285	0.00282025	0.99717975	0.24658659
55	0.01124303	0.98875697	0.00276901	0.99723099	0.24628656
56	0.01105566	0.98894434	0.00271965	0.99728035	0.24599606
57	0.01087423	0.98912577	0.00267206	0.99732794	0.24572377
58	0.01069894	0.98930106	0.00262616	0.99737384	0.24546003
59	0.01052904	0.98947096	0.00258184	0.99741816	0.24521104
60	0.01036468	0.98963532	0.00253904	0.99746096	0.24497037

CONCLUSIONS

The edges in the graph connect vertices of various degrees, which is characterized by quantities m_{ij}. For chemically interesting molecular graphs (with maximal degrees at most 4), the m_{ij}s can be represented by 10-tuples. In the present paper, theorems have been proved that show under which conditions monocyclic graph(s) exist for a given arbitrary 10-tuple. These theorems have enabled development of the algorithm that was applied to compare discriminative properties of the Zagreb and modified Zagreb indices.

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SAŽETAK

O egzistenciji monocikličkih molekula sa zadanim uvjetima na susjedstvo valencija: generirajući algoritam i njegova primjena u testiranju diskriminativnih svojstava Zagrebačkoga i modificiranoga Zagrebačkoga indeksa

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Susjedstva valencija (stupnjeva) u molekularnim grafovima (bez vodikovih atoma) su karakterizirana desetorkama brojeva m_{ij} gdje m_{ij} označava broj grana koje povezuju vrhove stupnjeva i i j. Pokazano je koje su desetorke kompatibilne s monocikličkim grafovima i dokazani matematički iskazi su rabljeni za usporedbu diskriminativnih svojstava Zagrebačkoga i modificiranoga Zagrebačkoga indeksa.