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On acyclic molecular graphs with prescribed numbers of edges that connect vertices with given degrees

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We find a necessary and sufficient conditions on a sequence

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

for the existence of an acyclic molecular graph G such that exactly m_{ij} edges connect vertices of degree i and j. We use this result together with two additional results to make an algorithm that generates all the sequences

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

such that a molecular acyclic graph exists with exactly m_{ij} edges connecting vertices of degree i and j. This algorithm is utilized to compare discriminative properties of the Zagreb index and the modified Zagreb index, and it is found that the modified Zagreb index is more discriminative then the Zagreb index.

KEY WORDS: acyclic graph, molecular graph, algorithm, generator, discriminitavity, topological index, molecular descriptor, Zagreb index, modified Zagreb index

1. Introduction and main results

The algorithmic graph theory is very ubiquitious part of graph theory which becomes more and more important as computers play a bigger and bigger role in all aspects of human life [1]. Also, the connection between chemistry and graph theory is very important. Applications of graph theory in chemistry are very important, and they strongly influence the development of chemistry [2]. The aim of this paper is to present one very interesting mathematical result, describe how it can be utilized in the development of a very useful

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algorithm, and give an example of its use by solving an interesting chemical problem.

Molecules are conveniently described as graphs [3,4] and there is an intuitively very clear correspondence between chemical and graph-theoretical notions: atoms are represented by vertices and chemical bonds by edges. The ability of atoms to make chemical bonds, i.e. their valences, are equivalent to notion of vertex degrees in graph.

Since, we model molecules by graphs, we are interested only in connected graphs with maximal degree at most four and with a finite number of vertices. In this paper we restrict our attention to the acyclic graphs. Since for each such graph there is an isomorphic graph with all vertices in $\mathbb{N}$ (where $\mathbb{N}$ is the set of natural numbers), it is sufficient to observe the set $\mathcal{T}$ of all connected acyclic graphs with maximal degree at most four and for which all vertices belong to $\mathbb{N}$ (requirement that all vertices belong to $\mathbb{N}$ is just a technical detail that enables us have set $\mathcal{T}$ instead of class of all connected acyclic graphs with maximal degree at most four, the set $\mathbb{N}$ could be replaced by any other infintensimal set). Basically, our results cover the family of alkanes and they are mainly intended for the study of this family of molecules.

To each graph $G \in \mathcal{T}$ 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 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: $\mathcal{T} \to \mathbb{N}_0^{10}$ is defined. The set $\mathbb{N}_0$ is the set of all natural number together with number 0.

It can be easily seen that this function is not a surjection, e.g. there is no graph $G \in \mathcal{T}$ such that

$$m_{11} = 3 \text{ and } m_{12} = m_{13} = m_{14} = m_{22} = m_{23} = m_{24} = m_{33} = m_{34} = m_{44} = 0.$$

Since, the sequences that are in $\mu(\mathcal{T})$ play an important role in chemistry, while sequences in $\mathbb{N}_0^{10} \setminus \mu(\mathcal{T})$ are of no interest to chemistry what so ever, it is very important to find the set $\mu(\mathcal{T})$. Or, equivalently, 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 $\mu(\mathcal{T})$. In the second section of paper, we find these necessary and sufficient conditions as the main theorem of this paper.

In order to utilize this theorem, for various chemical applications, we need to find a fast algorithm that generates, for prescribed $n \in \mathbb{N}$, all the sequences $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$ that satisfy the conditions of this theorem such that

$$m_{11} + m_{12} + m_{13} + m_{14} + m_{22} + m_{23} + m_{24} + m_{33} + m_{34} + m_{44} = n - 1.$$

Of course, on first sight, this seems easy. We could simply generate all such possible sequences $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$ by a well known algorithm given in [5] and then test them by the criterium of our theorem.

Unfortunately, the number of combinations that need to be checked becomes to large as n grows. For instance, when $n = 70$, the number of combinations is

$$\binom{70+9}{9} = 205\,811\,513\,765,$$

which is too large. Therefore, we need to find a much more sophisticated algorithm. We do that in the third section. In this way, we have analyzed all acyclic molecular graphs.

Explicit construction and analysis, without usage of our theorem, of these trees would be extremely inefficient and even the best computers would be useless for large values ($\geqslant 40$) of n. The efficiency of algorithms is probably the most important topic of algorithmic graph theory [1,6,7].

This algorithm can find very important applications in chemistry. As an example, we give one very important chemical result.

Fifty-six years ago, chemists [8] noticed that information given by graph can be compressed in a single number, a so called molecular descriptor. Of course, there is an infinite number of ways to do this and only those descriptors that correlate well with physical, chemical and biological properties of molecules are of interest to study. Such indices have found enormous application in Quantitive Structure Property Relationship (QSPR) and Quantitive Structure Activity Relationship (QSAR) and other studies, and for an overview the reader is referred to a recent monograph [9]. Many of these indices are uniquely defined by a sequence $\mu(G) = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$. There are many important indices defined in this way. One of the most famous such indices is the Zagreb index [10], defined by:

$$M_2(G) = \sum_{e \in E(G)} v_1(e)\, v_2(e),$$

where $v_1(e)$ and $v_2(e)$ denote valences of vertices incident to an edge e. It is found that this index has a large number of important properties [11]. In more condensed form this can be written as:

$$M_2(G) = m_{11} + 2m_{12} + 3m_{13} + 4m_{14} + 4m_{22} + 6m_{23} + 8m_{24} + 9m_{33} + 12m_{34} + 16m_{44}.$$

Recently, in [12], the following modification of Zagreb index was proposed:

$${}^*M_2(G) = \sum_{e \in E(G)} (v_1(e)\, v_2(e))^{-1}.$$

This index is called modified Zagreb index. It can also be rewritten as:

$${}^*M_2(G) = m_{11} + \tfrac{1}{2}m_{12} + \tfrac{1}{3}m_{13} + \tfrac{1}{4}m_{14} + \tfrac{1}{4}m_{22} + \tfrac{1}{6}m_{23} + \tfrac{1}{8}m_{24} + \tfrac{1}{9}m_{33} + \tfrac{1}{12}m_{34} + \tfrac{1}{16}m_{44}.$$

Obviously if two graphs G and G' have equal sequences $\mu(G)$ and $\mu(G')$ they can not be discriminated by any of these two indices. So, it sufficient to analyze how well these indices distinguish sequences $m, m' \in \mu(\mathcal{T})$. Using an algorithm developed in the third section, we do this in the fourth section.

2. Necessary and sufficient conditions on m_{ij} for existence of acyclic molecular graph

In this section we prove the most important theorem in this paper. Namely, we give a necessary and sufficient conditions on numbers $m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}$ and m_{44} such that

$$(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in \mu(\mathcal{T}).$$

We use standard graph theory terms and notation given in [13,14]. Also, define the function $\mu: \mathcal{T} \to \mathbb{N}_0^{10}$ by

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

if and only if exactly m_{ij} edges connect vertices with degrees i and j in graph G for each $1 \leqslant i \leqslant j \leqslant 4$ and We also define functions $\mu_{ij}: \mathcal{T} \to \mathbb{N}_0$, for each $1 \leqslant i \leqslant j \leqslant 4$, by

$$\mu_{ij}(G) = m_{ij}$$

if and only if exactly m_{ij} edges connect vertices with degrees i and j. By P_n, we denote a path with n vertices.

Let us prove the main theorem of this paper:

Theorem 1. Let $m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in \mathbb{N}_0^{10}$. There is an acyclic molecular graph G with at least two vertices such that $\mu(G) = m$ if and only if one of the following statements holds:

(1) $m = (1, 0, 0, 0, 0, 0, 0, 0, 0, 0)$

(2) $m = (0, 2, 0, 0, m_{22}, 0, 0, 0, 0, 0)$

(3) $(m_{11} = 0)$ and $(n_2, n_3, n_4 \in \mathbb{N}_0)$ and $(q \geqslant 0)$ and $(m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1)$ and $[(m_{12} + m_{23} + m_{24} \neq 0)$ or $(m_{22} = 0)]$ and one of the following holds:

(3.1) $(m_{44} \leqslant n_4 - 1)$ and $(m_{33} \leqslant n_3 - 1)$ and $(q + m_{33} - m_{24} \leqslant n_3 - 1)$ and $(q + m_{44} - m_{23} \leqslant n_4 - 1)$

(3.2) $(n_3 = 0)$

(3.3) $(n_4 = 0)$

where

$$\begin{aligned} n_2 &= (m_{12} + 2m_{22} + m_{23} + m_{24})/2, \\ n_3 &= (m_{13} + m_{23} + 2m_{33} + m_{34})/3, \\ n_4 &= (m_{14} + m_{24} + m_{34} + 2m_{44})/4, \\ q &= (m_{23} + m_{24} - m_{12})/2. \end{aligned}$$

Proof. First let us prove sufficiency. Suppose that there is an acyclic molecular graph G such that $\mu(G) = m$. If $m = (1, 0, 0, 0, 0, 0, 0, 0, 0, 0)$ or $m = (0, 2, 0, 0, m_{22}, 0, 0, 0, 0, 0)$, the claim is trivial. So suppose that $m \neq (1, 0, 0, 0, 0, 0, 0, 0, 0, 0)$ and $m \neq (0, 2, 0, 0, m_{22}, 0, 0, 0, 0, 0)$. Since G is connected, it follows that $m_{11} = 0$ and that $m_{12}+m_{23}+m_{24} \neq 0$ or $m_{22} = 0$. Note that n_i is the number of vertices of degree i in graph G for $i = 2, 3, 4$, so naturally $n_2, n_3, n_4 \in \mathbb{N}$.

Now, let us observe the set $\mathcal{P}$ of all paths in G with the following proerties:

(1) The length of each path is at least 2;

(2) All interior vertices have degrees 2;

(3) Exterior vertices have degrees different then 2.

Denote the number of such paths by p. Note that $p = (m_{12} + m_{23} + m_{24})/2$. Since $m \neq (0, 2, 0, 0, m_{22}, 0, 0, 0, 0, 0)$ and G is connected, it follows that there is no such paths with both terminal vertices of degree 1. Therefore $p \leqslant m_{23} + m_{24}$. Each edge connecting vertices of degree 1 and 2 belongs to one of these paths, so $p \geqslant m_{12}$. Therefore $m_{12} \leqslant m_{23} + m_{24}$ and consequently $q \geqslant 0$. Denote by $\mathcal{P}'$ set of these paths that have both endvertices of degree 3 or 4. Note that $\mathcal{P}$ has exactly $(m_{12} + m_{23} + m_{24})/2 - m_{12} = q$ elements. Let G' be a graph obtained from G by following operations:

(1) Delete all vertices of degree 1 with their adjacent edges and all edges and vertices except terminal vertex of degree 3 and 4 of all paths in $\mathcal{P} \setminus \mathcal{P}'$.

(2) Contract all paths in $\mathcal{P}'$ to a single edge connecting their terminal vertices.

Note that G' is a tree and it has $n_3 + n_4$ vertices and $m_{33} + m_{34} + m_{44} + q$ edges. It follows that

$$m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1.$$

It remains to prove that one of the statements (3.1)–(3.3) holds.

If there are no vertices of degree 3 in G or if there are no vertices of degree 4 in G, the claim is trivial, hence suppose $n_3, n_4 \neq 0$. Denote by N_3 the set of vertices of degree 3 and by N_4 the set of vertices of degree 4. Denote by $G[X]$

the subgraph of G induced by X. The graph $G[N_3]$ is an acyclic graph with m_{33} edges, hence $m_{33} \leqslant n_3 - 1$. Analogously, the graph $G[N_4]$ is an acyclic graph with m_{44} edges, therefore $m_{44} \leqslant n_4 - 1$.

Denote by $\mathcal{P}'_{33}$ set of all paths in $\mathcal{P}'$ such that their terminal vertices have degree 3; by $\mathcal{P}'_{34}$ set of all paths in $\mathcal{P}'$ such that they have one terminal vertex of degree 3 and other of degree 4; and by $\mathcal{P}'_{44}$ set of all paths in $\mathcal{P}'$ such that their terminal vertices have degree 4. Of course, $\mathcal{P}' = \mathcal{P}'_{33} \cup \mathcal{P}'_{34} \cup \mathcal{P}'_{44}$. Note that $\mathcal{P}'_{33}$ has at least $q - m_{24}$ elements and that $\mathcal{P}'_{44}$ has at least $q - m_{23}$ elements.

Let G'' be a graph obtained by contraction of all edges in $\mathcal{P}'_{33}$ to a single edge connecting their terminal vertices. Note that $G''[N_3]$ is an acyclic graph with n_3 vertices and $\left|\mathcal{P}'_{33}\right| + m_{33}$ edges. Therefore,

$$(q - m_{24}) + m_{33} \leqslant \left|\mathcal{P}'_{33}\right| + m_{33} \leqslant n_3 - 1.$$

Now, let G''' be a graph obtained by contraction of all edges in $\mathcal{P}'_{44}$ to a single edge connecting their terminal vertices. Note that $G''[N_4]$ is an acyclic graph with n_4 vertices and $\left|\mathcal{P}'_{44}\right| + m_{44}$ edges. Therefore,

$$(q - m_{24}) + m_{33} \leqslant \left|\mathcal{P}'_{33}\right| + m_{33} \leqslant n_3 - 1.$$

Now, let us prove necessity. Denote $n_1 = m_{11} + m_{12} + m_{13} + m_{14}$. We need to prove the following five statements:

(1) If $m = (1, 0, 0, 0, 0, 0, 0, 0, 0, 0)$, then there is an acyclic molecular graph G such that $\mu(G) = m$.

(2) If $m = (0, 2, 0, 0, m_{22}, 0, 0, 0, 0, 0)$, then there is an acyclic molecular graph G such that $\mu(G) = m$.

(3) If

$$(m_{11} = 0) \text{ and } (n_2, n_4 \in \mathbb{N}) \text{ and } (q \geqslant 0) \text{ and } (m_{44} + q = n_4 - 1) \text{ and } [(m_{12} + m_{24} \neq 0) \text{ or } (m_{22} = 0)] \text{ and } (n_3 = 0),$$

then there is an acyclic molecular graph G such that $\mu(G) = m$.

(4) If

$$(m_{11} = 0) \text{ and } (n_2, n_3 \in \mathbb{N}) \text{ and } (q \geqslant 0) \text{ and } (m_{33} + q = n_3 - 1) \text{ and } [(m_{12} + m_{23} \neq 0) \text{ or } (m_{22} = 0)] \text{ and } (n_4 = 0)$$

then there is an acyclic molecular graph G such that $\mu(G) = m$.

(5) If

$(n_3 \neq 0)$ and $(n_4 \neq 0)$ and $(m_{11} = 0)$ and $(n_2, n_3, n_4 \in \mathbb{N})$ and $(q \geqslant 0)$ and $(m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1)$ and $[(m_{12} + m_{23} + m_{24} \neq 0)$ or $(m_{22} = 0)]$ and $(m_{44} \leqslant n_4 - 1)$ and $(m_{33} \leqslant n_3 - 1)$ and $(q + m_{33} - m_{24} \leqslant n_3 - 1)$ and $(q + m_{44} - m_{23} \leqslant n_4 - 1)$

then there is an acyclic molecular graph G such that $\mu(G) = m$.

Let us prove them:

(1) We have $\mu(P_2) = m$.

(2) We have $\mu\left(P_{m_{22}+2}\right) = m$.

(3) Define set E_1 by

$$E_1 = \begin{cases} \left\{z_1 z_2,\, z_2 z_3,\, \dots,\, z_{n_4-1} z_{n_4}\right\} & m_{24} - m_{12} = 0, \\ \left\{\begin{array}{c} z_1 y_1,\, y_1 z_2,\, z_2 y_2,\, y_2 z_3,\, \dots, \\ z_{n_2-m_{12}} y_{n_2-m_{12}},\, y_{n_2-m_{12}} z_{n_2-m_{12}+1}, \\ z_{n_2-m_{12}+1} z_{n_2-m_{12}+2}, \\ z_{n_2-m_{12}+2} z_{n_2-m_{12}+3},\, \dots,\, z_{n_4-1} z_{n_4}, \end{array}\right\}, & \begin{array}{c} m_{22} = 0 \text{ and} \\ m_{24} - m_{12} \neq 0, \end{array} \\ \left\{\begin{array}{c} z_1 y_1,\, y_1 y_2,\, y_2 y_3,\, \dots,\, y_{m_{22}} y_{m_{22}+2},\, y_{m_{22+1}} z_2, \\ z_2 y_{m_{22}+2},\, y_{m_{22}+2} z_3,\, \dots, \\ z_{n_2-m_{22}-m_{12}} y_{n_2-m_{12}},\, y_{n_2-m_{12}} z_{n_2-m_{22}-m_{12}+1}, \\ z_{n_2-m_{22}-m_{12}+1} z_{n_2-m_{22}-m_{12}+2}, \\ z_{n_2-m_{22}-m_{12}+2} z_{n_2-m_{22}-m_{12}+3},\, \dots,\, z_{n_4-1} z_{n_4}, \end{array}\right\}, & \begin{array}{c} m_{22} \neq 0, \text{ and} \\ m_{24} - m_{12} \neq 0, \end{array} \end{cases}$$

sequence s_1 by

$$s_1 = \left(z_1, z_1, z_1, z_2, z_2, z_3, z_3, \dots, z_{n_4-1}, z_{n_4-1}, z_{n_4}, z_{n_4}, z_{n_4}\right);$$

sequence s_2 by

$$s_2 = \begin{cases} \left(x_1, x_2, \dots, x_{n_1}\right), & m_{12} = 0 \\ \left(\begin{array}{c} y_{n_2-m_{12}+1}, y_{n_2-m_{12}+2}, y_{n_2-m_{12}+3}, \dots, y_{n_2}, \\ x_1, x_2, \dots, x_{n_1-m_{12}} \end{array}\right), & \begin{array}{c} m_{12} \neq 0 \text{ and}, \\ \left(\begin{array}{c} m_{22} = 0 \text{ or} \\ m_{24} - m_{12} \neq 0 \end{array}\right), \end{array} \\ \left(\begin{array}{c} y_{n_2-m_{12}+1}, y_{n_2-m_{12}+2}, y_{n_2-m_{12}+3}, \dots, y_{n_2-m_{22}}, \\ x_1, x_2, \dots, x_{n_1-m_{12}} \end{array}\right), & \begin{array}{c} m_{12} \neq 0 \text{ and} \\ \left(\begin{array}{c} m_{22} \neq 0 \text{ and} \\ m_{24} - m_{12} = 0 \end{array}\right), \end{array} \end{cases}$$

sequence s_3 by

$$s_3 = \begin{cases} \emptyset, & m_{12} = 0, \\ \left(x_{n_1-m_{12}+1}, x_{n_1-m_{12}+2}, \dots, x_{n_1}\right) & m_{12} \neq 0, \end{cases}$$

where $\emptyset$ denotes the empty sequence. Now, define set E_2 by

$$E_2 = \left\{(s_1)_i\,(s_2)_i\colon 1 \leqslant i \leqslant |s_1|\right\}$$

set E_3 by

$$E_3 = \begin{cases} \emptyset, & m_{12} = 0 \\ \left\{(s_2)_i\,(s_3)_i\colon 1 \leqslant i \leqslant m_{12}\right\}, & \begin{array}{c} m_{12} \neq 0 \text{ and,} \\ \left(\begin{array}{c} m_{22} = 0 \text{ or} \\ m_{24} - m_{12} \neq 0 \end{array}\right), \end{array} \\ \begin{array}{c} \left\{(s_2)_i\,(s_3)_i\colon 2 \leqslant i \leqslant m_{12}\right\} \cup \\ \left\{\begin{array}{c} y_{n_2-m_{12}+1}y_{n_2-m_{22}},\, y_{n_2-m_{22}}y_{n_2-m_{22}+1}, \\ y_{n_2-m_{22}+1}y_{n_2-m_{22}+2}, \ldots, \\ y_{n_2-1}y_{n_2},\, y_{n_2}x_{n_2-m_{12}+1} \end{array}\right\}, \end{array} & \begin{array}{c} m_{12} \neq 0 \text{ and} \\ \left(\begin{array}{c} m_{22} \neq 0 \text{ and} \\ m_{24} - m_{12} = 0 \end{array}\right). \end{array} \end{cases}$$

Graph G given by

$$\begin{aligned} V(G) &= \left\{x_1, x_2, \ldots, x_{n_1}, y_1, y_2, \ldots, y_{n_2}, \ldots, z_{n_1}, \ldots, z_{n_4}\right\}, \\ E(G) &= E_1 \cup E_2 \cup E_3 \end{aligned}$$

has the required properties.

(4) This case can be proved by complete analogy with the previous case.

(5) We have

$$\max\{0, q - m_{24}\} \leqslant \min\left\{q, n_4 + m_{23} - q - m_{44} - 1, \left\lfloor \frac{m_{23}}{2} \right\rfloor, n_3 - 1 - m_{33}\right\}.$$

Therefore, there is $x \in \mathbb{N}_0$ such that

$$\max\{0, q - m_{24}\} \leqslant x \leqslant \min\left\{\begin{array}{c} q, n_4 + m_{23} - q - m_{44} - 1, \\ \left\lfloor \frac{m_{23}}{2} \right\rfloor, n_3 - 1 - m_{33} \end{array}\right\}. \tag{1}$$

Now, it follows that

$$\max\{x + q - m_{23}, 0\} \leqslant \min\{x + m_{24} - q, n_4 - m_{44} - 1, q - x\}.$$

This implies that there is $z \in \mathbb{N}_0$ such that

$$\max\{x + q - m_{23}, 0\} \leqslant z \leqslant \min\{x + m_{24} - q, n_4 - m_{44} - 1, q - x\}$$

or equivalently that

$$x + q - m_{23} \leqslant z, \tag{2}$$
$$0 \leqslant z,$$
$$z \leqslant x + m_{24} - q, \tag{3}$$
$$z \leqslant n_4 - m_{44} - 1, \tag{4}$$
$$z \leqslant q - x.$$

Putting $y = q - x - z$. From the last inequality, it follows that $y \in \mathbb{N}_0$. Putting this in inequalities (1)–(4), we find that there are numbers $x, y, z \in \mathbb{N}_0$ such that

$$\begin{aligned} m_{33} + x &\leqslant n_3 - 1, \\ m_{44} + z &\leqslant n_4 - 1, \\ 2x + y &\geqslant m_{23}, \\ 2z + y &\leqslant m_{24}. \end{aligned}$$

Denote

$$\begin{aligned} m'_{13} &= m_{13} + (m_{23} - 2x - y), \\ m'_{14} &= m_{14} + (m_{24} - 2z - y), \\ m'_{33} &= m_{33} + x, \\ m'_{34} &= m_{34} + y, \\ m'_{44} &= m_{44} + z, \\ m' &= \left(0, 0, m'_{13}, m'_{14}, 0, 0, 0, m'_{33}, m'_{34}, m'_{44}\right). \end{aligned}$$

Note that

$$\begin{aligned} n_3 &= \frac{m'_{13} + 2m'_{33} + m'_{34}}{3}, \\ n_4 &= \frac{m'_{14} + m'_{34} + 2m'_{44}}{4}, \\ m'_{33} &\leqslant n_3 - 1, \\ m'_{44} &\leqslant n_4 - 1, \\ m'_{33} + m'_{34} + m'_{44} &= m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1. \end{aligned}$$

Let

$$V\left(G'\right) = \left\{a_1, \ldots, a_{n_3}, b_1, \ldots, b_{n_4}, c_1, \ldots, c_{m'_{13}}, d_1, \ldots, d_{m'_{14}}\right\}.$$

Distinguish two cases:

(1) $n_3 - m'_{33} \leqslant n_4 - m'_{44}$.

From

$$n_3 - m'_{33} \leqslant n_4 - m'_{44},$$

it follows that

$$1 + 2\left(n_3 - m'_{33} - 1\right) \leqslant \left(n_3 - m'_{33}\right) + \left(n_4 - m'_{44}\right) - 1$$

and from

$$n_3 + n_4 - 1 \leqslant m'_{33} + m'_{34} + m'_{44} + m'_{13},$$

it follows that

$$n_3 + n_4 - m'_{33} - m'_{44} - 1 \leqslant 3n_3 - 2m'_{33}.$$

Therefore,

$$1 + \underbrace{2 + \cdots + 2}_{(n_3 - m'_{33} - 1)\text{-times}} \leqslant \left(n_3 - m'_{33}\right) + \left(n_4 - m'_{44}\right) - 1 \leqslant \underbrace{3 + \cdots + 3}_{(n_3 - m'_{33} - 1)\text{-times}} + \left(m'_{33} + 3\right),$$

so there are numbers $p_1, \ldots, p_{n_3 - m_{33}}$ such that $1 \leqslant p_{n_3 - m'_{33}} \leqslant \left(m'_{33} + 3\right)$; $1 \leqslant p_i \leqslant 3$ for each $i = 1, \ldots, n_3 - m'_{33} - 1$ and

$$p_1 + \cdots + p_{n_3 - m_{33}} = \left(n_3 - m'_{33}\right) + \left(n_4 - m'_{44}\right) - 1.$$

Define the following multisets

$$A' = \left\{a_{n_3 - m'_{33}}, a_{n_3 - m'_{33}}, a_{n_3 - m'_{33} + 1}, a_{n_3 - m'_{33} + 2, \ldots,} a_{n_3 - 1}, a_{n_3}, a_{n_3}\right\},$$
$$A = A' \cup \left\{a_1, a_1, a_1, a_2, a_2, a_2, \ldots, a_{n_3 - m'_{33} - 1}, a_{n_3 - m'_{33} - 1}, a_{n_3 - m'_{33} - 1}\right\},$$
$$B' = \left\{\begin{matrix} b_{n_4 - m'_{44}}, b_{n_4 - m'_{44}}, b_{n_4 - m_{44}}, b_{n_4 - m_{44} + 1}, b_{n_4 - m'_{44} + 1}, b_{n_4 - m'_{44} + 2}, b_{n_4 - m'_{44} + 2}, \ldots \\ b_{n_4 - 1}, b_{n_4 - 1}, b_{n_4}, b_{n_4}, b_{n_4} \end{matrix}\right\},$$
$$B = B' \cup \left\{b_1, b_1, b_1, b_1, b_2, b_2, b_2, b_2, \ldots, b_{n_4 - m'_{44} - 1}, b_{n_4 - m'_{44} - 1}, b_{n_4 - m'_{44} - 1}, b_{n_4 - m'_{44} - 1}\right\}.$$

Define sequence s_1 by

$$s_1 = \left(\underbrace{a_1, \ldots, a_1}_{p_1\text{-times}}, \underbrace{a_2, \ldots, a_2}_{p_2\text{-times}}, \ldots, \underbrace{a_{n_3 - m'_{33} - 1}, \ldots, a_{n_3 - m'_{33} - 1}}_{p_{n_3 - m'_{33} - 1}\text{-times}}, a_{i_1}, a_{i_2}, \ldots, a_{i_{p_{n_3 - m'_{33}}}}\right),$$

where multiset $\left\{a_{i_1}, a_{i_2}, \ldots, a_{i_{p_{n_3 - m'_{33}}}}\right\}$ is the submultiset of the multiset A.

Define sequence s_2 by

$$s_2 = \left(\begin{matrix} b_1, b_2, \ldots, b_{p_1}, b_{p_1}, b_{p_1 + 1}, \ldots, b_{p_1 + p_2 - 1}, b_{p_1 + p_2 - 1}, b_{p_1 + p_2}, \ldots, b_{p_1 + p_2 + p_3 - 2}, \ldots, \\ b_{\left(p_1 + \cdots + p_{n_3 - m'_{33} - 1}\right) - \left(n_3 - m'_{33} - 2\right)}, b_{\left(p_1 + \cdots + p_{n_3 - m'_{33} - 1}\right) - \left(n_3 - m'_{33} - 2\right) + 1}, \ldots, \\ b_{\left(p_1 + \cdots + p_{n_3 - m'_{33}}\right) - \left(n_3 - m'_{33} - 1\right)} \end{matrix}\right).$$

Now, let s_3 be any sequence such that elements of s_1 and s_3 form the multiset A and let s_4 be any sequence such that elements of s_4 and s_2 form the multiset B. Let

$$\begin{aligned} E\left(G'\right) = &\left\{a_{n_3 - m_{33}} a_{n_3 - m_{33} + 1}, \ldots, a_{n_3 - 1} a_{n_3}, b_{n_4 - m'_{44}} b_{n_{44} - m'_{44} + 1}, b_{n_4 - 1}, b_{n_4}\right\} \\ &\cup \left\{(s_1)_i \, (s_2)_i\,,\ i = 1, \ldots, n_3 + n_4 - 1\right\} \\ &\cup \left\{(s_3)_i \, c_i,\ i = 1, \ldots, m'_{33}\right\} \cup \left\{(s_4)_i \, d_i,\ i = 1, \ldots, m'_{33}\right\}. \end{aligned}$$

It can be easily seen that graph G' has the required properties.

(2) $n_3 - m_{33} \geqslant n_4 - m_{44}$.
This case can be solved in the completely analogous way as Case 1.
So, in both cases, we have graph G' such that $\mu\left(G'\right) = m'$. Choose arbitrary:

(1) x edges of graph G' that connect vertices of degree 3;

(2) y edges that connect vertices of degree 3 and 4;

(3) z edges that connect vertices of degree 4;

(4) $m_{23} - 2x - y$ edges that connect vertices of degree 1 and 3;

(5) $m_{24} - 2z - y$ edges that connect vertices of degree 1 and 4.

Replace each of the selected edges by a path with two edges and denote the graph obtained in this way by G''. Note that G'' is also an acyclic molecular graph and that

$$\begin{aligned}\mu\left(G''\right) &= (0, (m_{24} - 2z - y) + (m_{23} - 2x - y), m_{13}, m_{14}, 0, m_{23}, m_{24}, m_{33}, m_{34}) \\ &= (m_{11}, m_{12}, m_{13}, m_{14}, 0, m_{23}, m_{24}, m_{33}, m_{34}).\end{aligned}$$

If $m_{22} = 0$, it is sufficient to take $G = G''$ and we are done. So, suppose that $m_{22} \neq 0$. Then, $m_{12} + m_{23} + m_{24} \neq 0$. Take an arbitrary edge that connects one vertex of degree 2 and one vertex of degree different form 2. Replace this edge by a path with $m_{22} + 1$ edges and denote the resultant graph by G. Note that G is also a connected molecular graph and that

$$\mu(G) = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}),$$

so the claim is proved. □

From this theorem, there easily follows an algorithm that for a specified sequence $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34})$ checks whether it is

$$(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}) \in \mu(\mathcal{T}).$$

The algorithm expressed in C++ takes the form:

```
int testing( int m11, int m12, int m13, int m14, int m22, int m23, int m24,
                                          int m33, int m34, int m44)
{
   int n2, n3, n4, q;
   brt++;
   if ( (m11 == 1) && (m12 == 0) && (m13== 0) && (m14== 0)&&
(m22 == 0) &&
          ( m23 == 0) &&(m24 == 0) && (m33 == 0) && (m34 == 0)
&& (m44 == 0) )
```

```
        return 1;
    if ( (m11 == 0) && (m12 == 2) && (m13 == 0) && (m14 == 0) &&
        (m23 == 0) && (m24 == 0) && (m33 == 0) && (m34 == 0)
&& (m44 == 0) )
        return 1;
    if ( m11 != 0 )
        return 0;
    if ( (m12 + m23 + m24 == 0) && (m22 != 0) )
        return 0;
    n2 = ( m12 + 2 * m22 + m23 + m24 ) / 2;
    if ( 2 * n2 != m12 + 2 * m22 + m23 + m24 )
        return 0;
    n3 = ( m13 + m23 + 2 * m33 + m34 ) / 3;
    if ( 3 * n3 != m13 + m23 + 2 * m33 + m34 )
        return 0;
    n4 = ( m14 + m24 + m34 + 2 * m44 ) / 4;
    if ( 4 * n4 != m14 + m24 + m34 + 2 * m44 )
        return 0;
    if ( m33 + m34 + m44 + (m23 + m24 − m12) / 2 != n3 + n4 − 1 )
        return 0;
    if ( m23 + m24 − m12 < 0 )
        return 0;
    if ( n3 == 0 )
        return 1;
    if ( n4 == 0 )
        return 1;
    q = ( m23 + m24 − m12 ) / 2;
    if ( m44 > n4 − 1 )
        return 0;
    if ( m33 > n3 − 1 )
        return 0;
    if ( q > m24 + n3 − m33 − 1 )
        return 0;
    if ( q > m23 + n4 − m44 − 1 )
        return 0;
    return 1;
}
```

3. Generating algorithm

The aim of this section is to give a fast algorithm that generates, for prescribed $n \in \mathbb{N}$, all the sequences $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$

that satisfy the conditions of the last theorem such that

$$m_{11} + m_{12} + m_{13} + m_{14} + m_{22} + m_{23} + m_{24} + m_{33} + m_{34} + m_{44} = n - 1.$$

As, it is mentioned in the introduction, the algorithm that would be based only on the theorem 1, would not be efficient. Therefore, we give two more theorems.

Theorem 2. Let $n_1, n_2, n_3, n_4, n \in \mathbb{N}_0$. There is an acyclic molecular graph with n vertices such that n_1 vertices have degree 1; n_2 vertices have degree 2; n_3 vertices have degree 3; and n_4 vertices have degree 4; if and only if

$$n_1 + n_2 + n_3 + n_4 = n,$$
$$n_3 + 2n_4 = n_1 - 2.$$

Proof. First let us prove sufficiency. Suppose that G is an acyclic molecular graph with required properties. The first equation is trivial. Since G is a tree, we have

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2\left(n_1 + n_2 + n_3 + n_4 - 1\right)$$

and after a simple calculation, the claim follows.

Now, let us prove neccesity. Let n_1, n_2, n_3, n_4 and n satisfy the required properties. We explicitly construct graph with the required properties. We start with path $P_{n_2+n_3+n_4}$.Add to each of the first $n_3$vertices exactly one pendant vertex. Add to next $n_4$vertices exactly two pendand vertices and also add to first and last vertex one (more) pendant vertex. The resultant graph has the required properties. □

Now, we give an algorithm that, for prescribed $n > 3$, generates all sequences (n_1, n_2, n_3, n_4) such that there is a molecular acyclic graph with n vertices, with n_1 of them of degree 1, n_2 of them of degree 2, n_3 of them of degree 3, and n_4 of them of degree 4.

```
void g1 ( int n )
{
 int n1, n2, n3, n4;
 for ( n3=0; n3 <= (n - 2) / 2; n3++ )
       for (n4=0; n4 <= (n - 2 - 2 * n3) / 3; n4++ )
       {
            if ((n3 ==0) && (n4 ==0) )
            {
               n1=2;
               n2=n−2;
            }
```

```
        else
        {
           n1 =n3+2 * n4 + 2;
           n2 =n−n1−n3−n4;
        }
        x ( n1, n2, n3, n4 );
    }
}
```

Theorem 3. Let $n_1, n_2, n_3, n_4 \in \mathbb{N}_0$ be numbers such that there is an acyclic molecular graph G' with n_1 vertices of degree 1; n_2 vertices of degree 2; n_3 vertices of degree 3; and n_4 vertices of degree 4. Let $m_{33}, m_{34}, m_{44} \in \mathbb{N}_0$. Then there is an acyclic molecular graph G with n_1 vertices of degree 1; n_2 vertices of degree 2; n_3 vertices of degree 3 and n_4 vertices of degree 4 such that $\mu_{33}(G) = m_{33}$, $\mu_{34}(G) = m_{34}$ and $\mu_{44}(G) = m_{44}$ if and only if one of the following statements holds:

(1) $(n_3 = 0)$ and $(n_4 = 0)$ and $(m_{33} = 0)$ and $(m_{34} = 0)$ and $(m_{44} = 0)$.

(2) $(n_3 \neq 0)$ and $(n_4 = 0)$ and $(n_3 - n_2 - 1 \leqslant m_{33} \leqslant n_3 - 1)$ and $(m_{34} = 0)$ and $(m_{44} = 0)$.

(3) $(n_3 = 0)$ and $(n_4 \neq 0)$ and $(n_4 - n_2 - 1 \leqslant m_{44} \leqslant n_4 - 1)$ and $(m_{33} = 0)$ and $(m_{34} = 0)$.

(4) $(n_3 \neq 0)$ and $(n_4 \neq 0)$ and $(m_{33} \leqslant n_3 - 1)$ and $(m_{44} \leqslant n_4 - 1)$ and $\max \left\{ \begin{matrix} 0, n_3 + n_4 - 1 - \\ n_2 - m_{33} - m_{44} \end{matrix} \right\} \leqslant m_{34} \leqslant \min \left\{ \begin{matrix} 3n_3 - 2m_{33}, 4m_4 - 2m_{44}, \\ n_3 + n_4 - 1 - m_{33} - m_{44} \end{matrix} \right\}$.

Proof. First, let us prove sufficiency. Suppose that graph G with the required properties exists. Denote the set of vertices of degree i of graph G by N_i, $i = 1, 2, 3, 4$. Distinguish four cases:

(1) $n_3 = 0$ and $n_4 = 0$.
Trivially, $m_{33} = m_{34} = m_{44} = 0$.

(2) $n_3 \neq 0$ and $n_4 = 0$.

Trivially, $m_{34} = m_{44} = 0$. Since $G[N_3]$ is acyclic, it follows that $m_{33} \leqslant n_3 - 1$ and since $G[N_2 \cup N_3]$ is connected, it follows that

$$n_2 + n_3 - 1 \leqslant 2n_2 + m_{33},$$

which yields the claim.

(3) $n_3 = 0$ and $n_4 \neq 0$.

Trivially, $m_{33} = m_{34} = 0$. Since $G[N_4]$ is acyclic, it follows that $m_{44} \leqslant n_4 - 1$ and since $G[N_2 \cup N_4]$ is connected, it follows that

$$n_2 + n_4 - 1 \leqslant 2n_{22} + m_{44},$$

which yields the claim.

(4) $n_3 \neq 0$ and $n_4 \neq 0$.

Obviously, $m_{34} \geqslant 0$. Since $G[N_3]$ is acyclic, it follows that $m_{33} \leqslant n_3 - 1$ and analogously since $G[N_4]$ is acyclic, it follows that $m_{44} \leqslant n_4 - 1$. Note that $G[N_2 \cup N_3 \cup N_4]$ is connected, so

$$n_2 + n_3 + n_4 - 1 \leqslant 2n_2 + m_{33} + m_{34} + m_{44},$$

which implies

$$n_3 + n_4 - 1 - n_2 - m_{33} - m_{44} \leqslant m_{34}.$$

Since

$$3n_3 = m_{13} + m_{23} + 2m_{33} + m_{34},$$
$$4n_4 = m_{14} + m_{24} + m_{34} + 2m_{44},$$

it follows that

$$m_{34} \leqslant 3n_3 - 2m_{33},$$
$$m_{44} \leqslant 4n_4 - 2m_{44}.$$

Since $G[n_3 + n_3]$ is acyclic, we have

$$m_{33} + m_{34} + m_{44} \leqslant n_3 + n_4 - 1,$$

which implies

$$m_{34} \leqslant n_3 + n_4 - 1 - m_{33} - m_{44}.$$

Now, let us prove necessity. From theorem 1, it follows that it is sufficient to find $m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}$ and m_{24} such that one of the relations (1)–(3) of that theorem holds where

$$m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}),$$
$$n_1 = m_{11} + m_{12} + m_{13} + m_{14},$$
$$n_2 = (m_{12} + 2n_{22} + m_{23} + m_{24})/2,$$
$$n_3 = (m_{13} + m_{23} + 2n_{33} + m_{34})/3,$$
$$n_4 = (m_{14} + m_{24} + m_{34} + 2n_{44})/4,$$
$$q = (m_{23} + m_{24} - m_{12})/2.$$

Distinguish four cases:

(1) $(n_3 = 0)$ and $(n_4 = 0)$ and $(m_{33} = 0)$ and $(m_{34} = 0)$ and $(m_{44} = 0)$.

It is sufficient to take

$$m = (0, 2, 0, 0, n_2 - 1, 0, 0, 0, 0, 0)\,.$$

(2) $(n_3 \neq 0)$ and $(n_4 = 0)$ and $(n_3 - n_2 - 1 \leqslant m_{33} \leqslant n_3 - 1)$ and $(m_{34} = 0)$ and $(m_{44} = 0)$

Let

$$\begin{aligned}
&m_{11} = 0,\;\; m_{14} = 0,\;\; m_{24} = 0,\\
&m_{23} = \begin{cases} (n_3 - 1 - m_{33}) \cdot 2 & n_2 = n_3 - 1 - m_{33},\\ (n_3 - 1 - m_{33}) \cdot 2 + 1, & n_2 \neq n_3 - 1 - m_{33},\end{cases}\\
&m_{22} = \begin{cases} 0, & n_2 = n_3 - 1 - m_{33},\\ n_2 - (n_3 - 1 - m_{33}) - 1, & n_2 \neq n_3 - 1 - m_{33},\end{cases}\\
&m_{12} = \begin{cases} 0, & n_2 = n_3 - 1 - m_{33},\\ 1, & n_2 \neq n_3 - 1 - m_{33},\end{cases}\\
&m_{13} = 3n_3 - m_{23} - 2m_{33} - m_{34}.
\end{aligned}$$

Indeed,

$$\begin{aligned}
&n_1 = m_{11} + m_{12} + m_{13} + m_{14} \in \mathbb{N}_0,\\
&n_2 = (m_{12} + 2n_{22} + m_{23} + m_{24})\,/2 \in \mathbb{N}_0,\\
&n_3 = (m_{13} + m_{23} + 2n_{33} + m_{34})\,/3 \in \mathbb{N}_0,\\
&n_4 = (m_{14} + m_{24} + m_{34} + 2n_{44})\,/4 \in \mathbb{N}_0\\
&\qquad [(m_{12} + m_{23} + m_{24} \neq 0) \;\text{ or }\; (m_{22} = 0)]\,.
\end{aligned}$$

Note that

$$m_{13} = \begin{cases} n_3 + 2 & n_2 = n_3 - 1 - m_{33},\\ n_3 + 1, & n_2 \neq n_3 - 1 - m_{33},\end{cases}$$

so indeed $m_{ij} \geqslant 0$, for each $1 \leqslant i \leqslant 4,\; i \leqslant j \leqslant 4$. Note that $q = n_3 - 1 - m_{33}$ in each case and that $m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1$, so the claim is proved.

(3) $(n_3 = 0)$ and $(n_4 \neq 0)$ and $(n_4 - n_2 - 1 \leqslant m_{44} \leqslant n_4 - 1)$ and $(m_{33} = 0)$ and $(m_{34} = 0)$

Simple check shows it is sufficient to take

$$m_{11} = 0,\ \ m_{13} = 0,\ \ m_{23} = 0,$$

$$m_{24} = \begin{cases} (n_4 - 1 - m_{44}) \cdot 2, & n_2 = n_4 - 1 - m_{44}, \\ (n_4 - 1 - m_{44}) \cdot 2 + 1, & n_2 \neq n_4 - 1 - m_{44}, \end{cases}$$

$$m_{22} = \begin{cases} 0, & n_2 = n_4 - 1 - m_{44}, \\ n_2 - (n_4 - 1 - m_4) - 1, & n_2 \neq n_4 - 1 - m_{44}, \end{cases}$$

$$m_{12} = n_2 - 2m_{22} - m_{24},$$

$$m_{14} = 4n_4 - m_{24} - m_{34} - 2m_{44}.$$

(4) $(n_3 \neq 0)$ and $(n_4 \neq 0)$ and $(m_{33} \leqslant n_3 - 1)$ and $(m_{44} \leqslant n_4 - 1)$ and $\max\left\{\begin{matrix} 0, n_3 + n_4 - 1- \\ n_2 - m_{33} - m_{44} \end{matrix}\right\} \leqslant m_{34} \leqslant \min\left\{\begin{matrix} 3n_3 - 2m_{33}, 4m_4 - 2m_{44}, \\ n_3 + n_4 - 1 - m_{33} - m_{44} \end{matrix}\right\}.$

Note that

$$\max\{0, n_3 - 1 - m_{33} + m_{44} - 3n_4\} \leqslant \min\left\{\begin{matrix} 3n_3 - 2m_{33} - m_{34}, \\ \frac{n_3 + n_4 - 1 - m_{33} - m_{34}}{2} \end{matrix}\right\},$$

so there is $x \in \mathbb{N}_0$ such that

$$\max\{0, n_3 - 1 - m_{33} + m_{44} - 3n_4\} \leqslant x \leqslant \min\left\{\begin{matrix} 3n_3 - 2m_{33} - m_{34}, \\ \frac{n_3 + n_4 - 1 - m_{33} - m_{34}}{2}, \\ n_3 - 1 - m_{33} \end{matrix}\right\}.$$

It follows that

$$\max\left\{\begin{matrix} 0, x + n_4 - 1+ \\ m_{33} - m_{44} - 2n_3 \end{matrix}\right\} \leqslant \min\left\{\begin{matrix} n_3 + n_4 - 1 - x - m_{33} - m_{34} - m_{44}, \\ x - n_3 + 1 + m_{33} - m_{44} + 3n_4, \\ n_4 - 1 - m_{44} \end{matrix}\right\},$$

hence there is $z \in \mathbb{N}_0$ such that

$$\max\left\{\begin{matrix} 0, x + n_4 - 1+ \\ m_{33} - m_{44} - 2n_3 \end{matrix}\right\} \leqslant z \leqslant \min\left\{\begin{matrix} n_3 + n_4 - 1 - x - m_{33} - m_{34} - m_{44}, \\ x - n_3 + 1 + m_{33} - m_{44} + 3n_4, \\ n_4 - 1 - m_{44} \end{matrix}\right\}.$$

Put $y = n_3 + n_4 - 1 - x - z - m_{33} - m_{34} - m_{44}$. Note that $y \in \mathbb{N}_0$, so we have found numbers $x, y, z \in \mathbb{N}_0$ such that

$$\begin{aligned} 2x + y + (2m_{33} + m_{34}) &\leqslant 3n_3, \\ 2z + y + 2m_{44} + m_{34} &\leqslant 4n_4, \\ m_{33} + m_{34} + m_{44} + x + y + z &= n_3 + n_4 - 1, \\ x + y + z &\leqslant n_2, \\ x + m_{33} &\leqslant n_3 - 1, \\ z + m_{44} &\leqslant n_4 - 1. \end{aligned}$$

Let us prove that it is sufficient to take:

$$
\begin{aligned}
m_{11} &= 0\\
m_{23} &= \begin{cases} 2x+y, & \begin{bmatrix}(n_3+n_4-1=n_2+m_{33}+m_{34}+m_{44}) \text{ or}\\ (3n_3=2m_{33}+m_{34}+2x+y)\end{bmatrix},\\ 2x+y+1, & \begin{bmatrix}(n_3+n_4-1\neq n_2+m_{33}+m_{34}+m_{44}) \text{ and}\\ (3n_3\neq 2m_{33}+m_{34}+2x+y)\end{bmatrix},\end{cases}\\
m_{24} &= \begin{cases} 2z+y, & \begin{bmatrix}(n_3+n_4-1=n_2+m_{33}+m_{34}+m_{44}) \text{ or}\\ (3n_3\neq 2m_{33}+m_{34}+2x+y)\end{bmatrix},\\ 2z+y+1, & \begin{bmatrix}(n_3+n_4-1\neq n_2+m_{33}+m_{34}+m_{44}) \text{ and}\\ (3n_3=2m_{33}+m_{34}+2x+y)\end{bmatrix},\end{cases}\\
m_{22} &= \begin{cases} 0, & n_3+n_4-1=n_2+m_{33}+m_{34}+m_{44},\\ n_2-n_3-n_4+m_{33}+m_{34}+m_{44}, & n_3+n_4-1\neq n_2+m_{33}+m_{34}+m_{44},\end{cases}\\
m_{12} &= 2n_2-2m_{22}-m_{23}-m_{24},\\
m_{13} &= 3n_3-m_{23}-2m_{33}-m_{34},\\
m_{14} &= 4n_4-m_{24}-m_{34}-2m_{44}.
\end{aligned}
$$

Obviously, we have

$$
\begin{aligned}
n_1 &= m_{11}+m_{12}+m_{13}+m_{14}\in\mathbb{N}_0,\\
n_2 &= (m_{12}+2n_{22}+m_{23}+m_{24})/2\in\mathbb{N}_0,\\
n_3 &= (m_{13}+m_{23}+2m_{33}+m_{34})/3\in\mathbb{N}_0,\\
n_4 &= (m_{14}+m_{24}+m_{34}+2m_{44})/4\in\mathbb{N}_0,\\
&\quad [(m_{12}+m_{23}+m_{24}\neq 0) \text{ or } (m_{22}=0)].\\
m_{44} &\leqslant n_4-1,\\
m_{33} &\leqslant n_3-1,\\
m_{22}, m_{23}, m_{24} &\geqslant 0.
\end{aligned}
$$

Note that

$$
\begin{aligned}
m_{12} &= \begin{cases} 2n_2-(2x+y)-(2z+y), & n_3+n_4-1=n_2 +m_{33}+m_{34}+m_{44},\\ 2n_2-2(n_2-n_3-n_4+m_{33}+m_{34}+m_{44}) -(2x+y)-(2z+y)-1, & n_3+n_4-1\neq n_2 +m_{33}+m_{34}+m_{44}\end{cases}\\
&= \begin{cases} 2(n_3+n_4-1-m_{33}-m_{34}-m_{44}) -(2x+y)-(2z+y), & n_3+n_4-1=n_2 +m_{33}+m_{34}+m_{44}\\ 2n_2-2(n_2-n_3-n_4+m_{33}+m_{34}+m_{44}) -(2x+y)-(2z+y)-1, & n_3+n_4-1\neq n_2 +m_{33}+m_{34}+m_{44}\end{cases}
\end{aligned}
$$

$$= \begin{cases} 2(n_3+n_4-1-m_{33}-m_{34}-m_{44}-x-y-z), & \begin{matrix} n_3+n_4-1=n_2 \\ +m_{33}+m_{34}+m_{44} \end{matrix} \\ 2n_2-2n_2+2\begin{pmatrix} n_3+n_4-1-m_{33} \\ -m_{34}-m_{44}-x-y-z \end{pmatrix}+2-1, & \begin{matrix} n_3+n_4-1\neq n_2 \\ +m_{33}+m_{34}+m_{44} \end{matrix} \end{cases}$$

$$= \begin{cases} 0, & \begin{matrix} n_3+n_4-1=n_2 \\ +m_{33}+m_{34}+m_{44}, \end{matrix} \\ 1, & \begin{matrix} n_3+n_4-1\neq n_2 \\ +m_{33}+m_{34}+m_{44}, \end{matrix} \end{cases}$$

so indeed $m_{12} \geqslant 0$.

Also, we have

$$m_{13} = \begin{cases} 3n_3 - 2m_{33} - m_{34} - (2x+y), & n_3+n_4-1 = n_2+m_{33}+m_{34}+m_{44}, \\ 3n_3 - 2m_{33} - m_{34} - (2x+y+1), & \left[\begin{matrix} \begin{pmatrix} n_3+n_4-1 \neq n_2+m_{33} \\ +m_{34}+m_{44} \end{pmatrix} \text{ and} \\ (3n_3 \neq 2m_{33}+m_{34}+2x+y) \end{matrix} \right]. \end{cases}$$

In the first case, it directly follows that $m_{13} \geqslant 0$ and in the second case we would have $m_{13} < 0$ only if

$$3n_3 - 2m_{33} - m_{34} - 2x - y = 0$$

but this case is excluded.

We have

$$m_{14} = \begin{cases} 4n_4 - 2m_{44} - m_{34} - (2z+y), & n_3+n_4-1 = n_2+m_{33}+m_{34}+m_{44}, \\ 4n_4 - 2m_{44} - m_{34} - (2z+y), & \left[\begin{matrix} \begin{pmatrix} n_3+n_4-1 \neq n_2+m_{33} \\ +m_{34}+m_{44} \end{pmatrix} \text{ and} \\ (3n_3 = 2m_{33}+m_{34}+2x+y) \end{matrix} \right]. \end{cases}$$

In the first case, obviously $m_{14} \geqslant 0$ and in the second case we would have $m_{14} < 0$, only if

$$4n_4 - 2m_{44} - m_{34} - (2z+y) = 0$$

but then

$$1 = [3n_3 - 2m_{33} - m_{34} - 2x - y] + [4n_4 - 2m_{44} - m_{34} - (2z+y)] = 0,$$

which is a contradiction. Note that

$$q = \frac{m_{23}+m_{24}-m_{12}}{2} = x+y+z$$

in any case, so $q \geqslant 0$. Now, it easily follows that

$$m_{33}+m_{34}+m_{44}+q = n_3+n_4-1.$$

We also have

$$q+m_{33}-m_{24} = \begin{cases} x+y+z+m_{33} \\ \quad -(2z+y), & \left[\begin{matrix}(n_3+n_4-1=n_2+m_{33}+m_{34}+m_{44}) \text{ or} \\ (3n_3\neq 2m_{33}+m_{34}+2x+y)\end{matrix}\right] \\ x+y+z+m_{33} \\ \quad -(2z+y+1), & \left[\begin{matrix}(n_3+n_4-1\neq n_2+m_{33}+m_{34}+m_{44}) \text{ and} \\ (3n_3=2m_{33}+m_{34}+2x+y)\end{matrix}\right] \end{cases}$$
$$\leqslant x-z+m_{33}\leqslant x+m_{33}\leqslant n_3-1,$$
$$q+m_{44}-m_{23} = \begin{cases} x+y+z+m_{44} \\ \quad -(2x+y), & \left[\begin{matrix}(n_3+n_4-1=n_2+m_{33}+m_{34}+m_{44}) \text{ or} \\ (3n_3=2m_{33}+m_{34}+2x+y)\end{matrix}\right] \\ x+y+z+m_{44} \\ \quad -(2x+y+1), & \left[\begin{matrix}(n_3+n_4-1\neq n_2+m_{33}+m_{34}+m_{44}) \text{ and} \\ (3n_3\neq 2m_{33}+m_{34}+2x+y)\end{matrix}\right] \end{cases}$$
$$\leqslant z-x+m_{44}\leqslant z+m_{44}\leqslant n_4-1,$$

which proves the claim. □

From this theorem an algorithm follows:

```
void g2 ( int n1, int n2, int n3, int n4)
{
  int m33, m34, m44, gm, dm;
  brg2++;
  if ((n3 !=0) && (n4 !=0) )
  {
     for (m33 = 0; m33 < n3; m33++ )
          for (m44 = 0; m44 < n4; m44++ )
          {
               gm=min ( 3 * n3 - 2 * m33, 4 * n4 - 2 * m44,
                      n3 + n4 - 1- m33 - m44 );
               dm = max ( 0, n3+n4-1-n2-m33-m44 );
               if (dm <= gm )
                  for (m34=dm; m34 <= gm; m34++ )
                  g3 ( n1, n2, n3, n4, m33, m34, m44);
          }
  }
  else if ( (n3==0) && (n4 !=0) )
      {
          dm=max ( 0, n4-1-n2 );
          for ( m44=dm; m44 <= n4-1; m44++ )
               g3 ( n1, n2, n3, n4, 0, 0, m44 );
  }
else if ( (n3 != 0) && (n4==0) )
  {
     dm=max ( 0, n3-1-n2 );
```

```
    for ( m33=dm; m33 <= n3-1; m33++ )
        g3 ( n1, n2, n3, n4, m33, 0, 0 );
  }
else
    g3 ( n1, n2, n3, n4, 0, 0, 0 );
}
```

Combining the three algorithms that we have developed, an overall algorithm results which efficiently generates all sequences

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

with the required properties. This algorithm is developed in programming language C++ as a console application [15].

4. Application

The aim of this section is to utilize the previous algorithm. We compare discriminative properties of the Zagreb index and the modified Zagreb index.

Let n be a prescribed natural number. Denote by $\mathcal{M}_n$ the set of all sequences $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$ such that

$$(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in \mu(\mathcal{T}),$$
$$m_{11} + m_{12} + m_{13} + m_{14} + m_{22} + m_{23} + m_{24} + m_{33} + m_{34} + m_{44} = n - 1.$$

Let us define the functions $M_2', {}^*M_2'$: $\mathcal{M}_n \to \mathbb{R}$ by:

$$M_2'(\mu(G)) = M_2(G),$$
$${}^*M_2'(\mu(G)) = {}^*M_2(G).$$

We also define

$$\mathcal{P}_n = \{\{m_1, m_2\} : m_1, m_2 \in \mathcal{M}_n,\ m_1 \neq m_2\},$$
$$\mathcal{D}_n = \left\{\{m_1, m_2\} : m_1, m_2 \in \mathcal{M}_n,\ M_2'(m_1) \neq M_2'(m_2)\right\},$$
$${}^*\mathcal{D}_n = \left\{\{m_1, m_2\} : m_1, m_2 \in \mathcal{M}_n,\ {}^*M_2'(m_1) \neq {}^*M_2'(m_2)\right\},$$
$$\mathcal{I}_n = \left\{\{m_1, m_2\} : m_1, m_2 \in \mathcal{M}_n,\ M_2'(m_1) = M_2'(m_2)\right\},$$
$${}^*\mathcal{I}_n = \left\{\{m_1, m_2\} : m_1, m_2 \in \mathcal{M}_n,\ {}^*M_2'(m_1) = {}^*M_2'(m_2)\right\}.$$

The probability that a pair of sequences in $\mathcal{M}_n$ will be discriminated by the Zagreb index is $|\mathcal{D}_n|/|\mathcal{M}_n|$ and probability that they won't be discriminated is $|\mathcal{I}_n|/|\mathcal{M}_n|$. Analogously, probability that a pair of sequences in $\mathcal{M}_n$ will be discriminated by modified Zagreb index is $|{}^*\mathcal{D}_n|/|\mathcal{M}_n|$ and probability that they won't be discriminated is $|{}^*\mathcal{I}_n|/|\mathcal{M}_n|$.

Note that the probability that two sequences in $\mathcal{M}_n$ will be discriminated by Zagreb index (or the modified Zagreb index) is different then the probability that two graphs with n vertices will be discriminated by the same index.

Our findings about these indices are summarized by table:

n	$\lvert\mathcal{I}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert\mathcal{D}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert{}^*\mathcal{I}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert\mathcal{D}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert{}^*\mathcal{I}_n\rvert / \lvert\mathcal{I}_n\rvert$
1	0.00000000	1.00000000	0.00000000	1.00000000	$Notdefined$
2	0.00000000	1.00000000	0.00000000	1.00000000	$Notdefined$
3	0.00000000	1.00000000	0.00000000	1.00000000	$Notdefined$
4	0.00000000	1.00000000	0.00000000	1.00000000	$Notdefined$
5	0.00000000	1.00000000	0.00000000	1.00000000	$Notdefined$
6	0.00000000	1.00000000	0.00000000	1.00000000	$Notdefined$
7	0.05555556	0.94444444	0.02777778	0.97222222	0.50000000
8	0.02500000	0.97500000	0.02500000	0.97500000	1.00000000
9	0.05291005	0.94708995	0.02645503	0.97354497	0.50000000
10	0.04421769	0.95578231	0.02806122	0.97193878	0.63461538
11	0.04995592	0.95004408	0.02233324	0.97766676	0.44705882
12	0.04519107	0.95480893	0.02028768	0.97971232	0.44893112
13	0.04585303	0.95414697	0.01813922	0.98186078	0.39559471
14	0.04224314	0.95775686	0.01565289	0.98434711	0.37054264
15	0.04123140	0.95876860	0.01397686	0.98602314	0.33898590
16	0.03864243	0.96135757	0.01253796	0.98746204	0.32446094
17	0.03714156	0.96285844	0.01136024	0.98863976	0.30586323
18	0.03504758	0.96495242	0.01034063	0.98965937	0.29504548
19	0.03362712	0.96637288	0.00954999	0.99045001	0.28399656
20	0.03197768	0.96802232	0.00882092	0.99117908	0.27584610
21	0.03069701	0.96930299	0.00823175	0.99176825	0.26816130
22	0.02933097	0.97066903	0.00770969	0.99229031	0.26285154
23	0.02821589	0.97178411	0.00726120	0.99273880	0.25734429
24	0.02707898	0.97292102	0.00686171	0.99313829	0.25339605
25	0.02608397	0.97391603	0.00651173	0.99348827	0.24964498
26	0.02510826	0.97489174	0.00619568	0.99380432	0.24675863
27	0.02423443	0.97576557	0.00591502	0.99408498	0.24407528
28	0.02338357	0.97661643	0.00565763	0.99434237	0.24194886
29	0.02261631	0.97738369	0.00542743	0.99457257	0.23997846
30	0.02187699	0.97812301	0.00521399	0.99478601	0.23833196
31	0.02119807	0.97880193	0.00501989	0.99498011	0.23680874
32	0.02054734	0.97945266	0.00484023	0.99515977	0.23556493
33	0.01994472	0.98005528	0.00467515	0.99532485	0.23440559
34	0.01936536	0.98063464	0.00452104	0.99547896	0.23345996

n	$\lvert\mathcal{I}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert\mathcal{D}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert{}^*\mathcal{I}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert\mathcal{D}_n\rvert / \lvert\mathcal{M}_n\rvert$	$\lvert{}^*\mathcal{I}_n\rvert / \lvert\mathcal{I}_n\rvert$
35	0.01882740	0.98117260	0.00437898	0.99562102	0.23258541
36	0.01831065	0.98168935	0.00424536	0.99575464	0.23185205
37	0.01782702	0.98217298	0.00412095	0.99587905	0.23116308
38	0.01736337	0.98263663	0.00400394	0.99599606	0.23059710
39	0.01692768	0.98307232	0.00389430	0.99610570	0.23005499
40	0.01650910	0.98349090	0.00379068	0.99620932	0.22961127
41	0.01611414	0.98388586	0.00369330	0.99630670	0.22919632
42	0.01573485	0.98426515	0.00360083	0.99639917	0.22884437
43	0.01537506	0.98462494	0.00351339	0.99648661	0.22851238
44	0.01502938	0.98497062	0.00343036	0.99656964	0.22824398
45	0.01470078	0.98529922	0.00335153	0.99664847	0.22798324
46	0.01438454	0.98561546	0.00327634	0.99672366	0.22776799
47	0.01408312	0.98591688	0.00320487	0.99679513	0.22756836
48	0.01379284	0.98620716	0.00313650	0.99686350	0.22740028
49	0.01351537	0.98648463	0.00307123	0.99692877	0.22723943
50	0.01324787	0.98675213	0.00300875	0.99699125	0.22711225
51	0.01299172	0.98700828	0.00294897	0.99705103	0.22698816
52	0.01274441	0.98725559	0.00289158	0.99710842	0.22689011
53	0.01250716	0.98749284	0.00283660	0.99716340	0.22679778
54	0.01227793	0.98772207	0.00278369	0.99721631	0.22672319
55	0.01205753	0.98794247	0.00273286	0.99726714	0.22665172
56	0.01184442	0.98815558	0.00268394	0.99731606	0.22659921
57	0.01163924	0.98836076	0.00263683	0.99736317	0.22654693
58	0.01144057	0.98855943	0.00259140	0.99740860	0.22650966
59	0.01124903	0.98875097	0.00254762	0.99745238	0.22647491
60	0.01106345	0.98893655	0.00250532	0.99749468	0.22645051
61	0.01088423	0.98911577	0.00246448	0.99753552	0.22642697
62	0.01071045	0.98928955	0.00242500	0.99757500	0.22641478
63	0.01054243	0.98945757	0.00238683	0.99761317	0.22640192
64	0.01037934	0.98962066	0.00234986	0.99765014	0.22639799
65	0.01022149	0.98977851	0.00231409	0.99768591	0.22639506
66	0.01006816	0.98993184	0.00227942	0.99772058	0.22639838
67	0.00991957	0.99008043	0.00224581	0.99775419	0.22640156
68	0.00977514	0.99022486	0.00221321	0.99778679	0.22641171
69	0.00963504	0.99036496	0.00218158	0.99781842	0.22642094
70	0.00949874	0.99050126	0.00215085	0.99784915	0.22643560

It can be easily concluded that discriminative properties of the modified Zagreb index supersede properties of the Zagreb index.

References

[1] R.C. Read, Ann. Discrete Math. 55 (1993) 201.
[2] A.T. Balaban, Ann. Discrete Math. 55 (1993) 109.
[3] N. Trinajstić, *Chemical Graph Theory, 2nd revised ed. 1992* (CRC Press, Boca Raton, 1983).
[4] I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer-Verlag, Berlin, 1986).
[5] D.R. Kreher and D.R. Stinson, *Combinatorial Algorithms – Generation, Enumeration and Search* (CRC Press, Boca Raton, 1999).
[6] A. Gibbons, *Algorithmic Graph Theory* (Cambridge University Press, Cambridge, 1985).
[7] K.H. Rosen, *Handbook of Discrete and Combinatorial Mathematics* (CRC Press, Boca Raton, 1999).
[8] H. Wiener, and J. Am., Chem. Soc. 69 (1947) 17.
[9] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors* (Wiley–VCH, Weinheim, 2000).
[10] I. Gutman and N. Trinajstić, Chem. Phys. Lett. 17 (1972) 535.
[11] I. Gutman, B. Ruščić, N. Trinajstić and C. F. Wilcox Jr., J. Chem. Phys. 62 (1975) 3399.
[12] N. Trinajstić, On Modified Zagreb M_2 Index, reported at the MATH/CHEM/COMP 2002, Dubrovnik, June 24–29, 2002.
[13] D. Veljan, *Kombinatorna I Diskretna Matematika* (Algoritam, Zagreb, 2001).
[14] B. Bollobás, *Graph Theory* (Springer-Verlag, New York, 1979).
[15] I. Horton, Beginning Visual C++ 6 (Wrox Press Ltd, Birmingham, 2000).