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On Molecular Graphs with Valencies 1, 2 and 4 with Prescribed Numbers of Bonds*

Damir Vukičević[a,] and Ante Graovac[a,b]**

[a]*Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia*

[b]*The Ruđer Bošković Institute, P.O. Box 180, HR-10002 Zagreb, Croatia*

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In this paper, necessary and sufficient conditions are given for the existence of molecular graph(s) with the prescribed sequence m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}, where m_{ij} denotes the number of edges (bonds) connecting vertices (atoms) of degree i with vertices of degree j. The main result expressed as Theorem 1 covers the great variety of molecules with valencies 1, 2 and 4.

INTRODUCTION

Molecules are conveniently described by graph(s)[1–3] and there is an intuitive 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 valencies, are equivalent to the notion of vertex degrees in a graph.

Regarding the vertex degrees, all n vertices of G could be partitioned in n_1 of those having degree 1, n_2 having degree 2, *etc*., and obviously $n = n_1 + n_2 +$.... In this way, a unique sequence n_1, n_2.... is ascribed to each graph. The inverse problem, namely whether there are graph(s) with a prescribed n_1, n_2.... sequence is a well known and already solved problem in chemistry and graph theory.[4,5] Besides the vertex degrees, one could further characterize the connectivity in the graph by specifying how many edges m_{ij} connect vertices of degree i with vertices of degree j. Here again an inverse problem could be posed, namely whether there are graph(s) with a prescribed m_{ij} sequence. Such a question was raised by Gutman[6] and was declared to be a difficult one. Here, we answer the question, but only for those graphs whose vertex degrees are 1, 2, and 4, *i.e.*, we offer an answer to whether there are graph(s) with a prescribed sequence m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}. This paper gives the necessary and sufficient conditions for m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44} to ensure the existence of graph(s) having that sequence, and it reads as:

Theorem 1.

* Dedicated to Academician Nenad Trinajstić on the happy occasion of his 65[th] birthday.

** Author to whom correspondence should be addressed. (E-mail: vukicevi@pmfst.hr)

$$
\begin{aligned}
&\left\{ f\left(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}\right)=1 \right\} \Leftrightarrow \\
&\Leftrightarrow \left\{ \begin{array}{l}
\left[(m_{11}=1)\wedge(m_{12}=0)\wedge(m_{14}=0)\wedge(m_{22}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee \\
\left[(m_{11}=0)\wedge(m_{12}=0)\wedge(m_{14}=0)\wedge(m_{22}\geq 3)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee \\
\left[(m_{11}=0)\wedge(m_{12}=2)\wedge(m_{14}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee \\
\left\{ \left\{ \begin{array}{l}
\left\{ \begin{array}{l}
(m_{11}=0)\wedge\left[(m_{22}=0)\vee(m_{12}>0)\right]\wedge(m_{14}+m_{12}=4) \\
\wedge(m_{12}=m_{24})\wedge(m_{44}=0)
\end{array} \right\} \vee \\
\left\{ \begin{array}{l}
(m_{11}=0)\wedge\left[(m_{22}=0)\vee\left[(m_{12}+m_{24}>0)\right]\right]\wedge(m_{12}\leq m_{24})\wedge \\
\left[\begin{array}{l}
\left(\frac{m_{14}+m_{24}+2m_{44}}{4}\in\mathbb{N}\right)\wedge\left(\frac{m_{24}-m_{12}}{2}\in\mathbb{N}_0\right)\wedge \\
\left(\frac{m_{14}+m_{24}+2m_{44}}{4}-1-\frac{m_{24}-m_{12}}{2}\leq m_{44}\leq\left(\frac{\frac{m_{14}+m_{24}+2m_{44}}{4}}{2}\right)\right) \\
\wedge\left(\frac{m_{14}+m_{24}+2m_{44}}{4}\geq 2\right)
\end{array} \right]
\end{array} \right\}
\end{array} \right\} \right\}
\end{array} \right\}
\end{aligned}
\tag{1}
$$

THE MAIN RESULT

Let $m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44} \in \mathbb{N}_0$. The aim of this paper is to determine if there is a simple connected graph G such that each vertex in G has degree 1, 2 or 4, and such that there are m_{ij} edges that connect vertices of degree i with vertices of degree j.

Formally, the existence could be described by function f defined by:

$$f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1 \tag{2}$$

if and only if there is a simple connected graph(s) G such that each vertex in G has degree 1, 2 or 4, and such that there are m_{ij} edges that connect vertices of degree i with vertices of degree j. Otherwise, one puts:

$$f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 0. \tag{3}$$

We need the following notation. Let G be a graph. By $d_G(x)$ we denote the degree of vertex x in G and by $N_G(x)$ the set of neighbors of vertex x in G. Let V(G) denote the set of vertices of G. For $V' \subseteq V$ a subgraph of G induced by V' is graph G' such that $V(G') = V'$ and edges of G' are the edges of G with their both endvertices in V'.

Let i, j be any natural numbers such that $i \leq j$. Denote by μ_{ij}(G) the number of edges in a given G that connect vertices of degrees i and j. The basic problem to be answered in this paper is to find whether μ_{ij}'s coincide with a prescribed sequence $m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}$. The answer is given by Theorem 1.

PROOF OF THEOREM 1

We start with a few Lemmas:

Lemma 1. – Suppose that $m_{11} > 0$. Then:

$$f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1. \tag{4}$$

if and only if $m_{11} = 1$, $m_{12} = 0$, $m_{14} = 0$, $m_{22} = 0$, $m_{24} = 0$, $m_{44} = 0$.

Proof: The condition that the graph must be connected implies the claim.

Obviously, this Lemma reflects the fact that there is only one connected graph with adjacent vertices of degree 1, which graph is called the complete graph K_2 or path P_2.

Lemma 2. – Suppose that $m_{22} > 0$ and $m_{11} = 0$. Then:

$$
\begin{aligned}
&\{f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1\} \Leftrightarrow \\
&\Leftrightarrow \left[\begin{array}{l}
((m_{12}+m_{24}>0)\wedge(f(m_{11}, m_{12}, m_{14}, 0, m_{24}, m_{44})=1))\vee \\
((m_{12}=0)\wedge(m_{14}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\wedge(m_{22}\geq 3))
\end{array} \right].
\end{aligned}
\tag{5}
$$

Proof: Suppose that we have $m_{12} + m_{24} \in \mathbb{N}$ and

$$f(0, m_{12}, m_{14}, 0, m_{24}, m_{44}) = 1. \tag{6}$$

Then there is a simple connected graph G such that each vertex in G has one of the following degrees 1, 2, 4, and such that $\mu_{11}(G) = m_{11}$, $\mu_{12}(G) = m_{12}$, $\mu_{14}(G) = m_{14}$, $\mu_{22}(G) = m_{22}$, $\mu_{24}(G) = m_{24}$, $\mu_{44}(G) = m_{44}$. Note that there is a vertex x such that $d_G(x) = 2$, because $m_{12} + m_{24}$

$\in \mathbb{N}$. Let denote $N_G(x) = \{y, z\}$ and let G be the following graph:

$$V(G') = (V(G) \setminus \{x\}) \cup \{v_0, v_1, v_2, ..., v_{m_{22}-1}, v_{m_{22}}\}$$

$$E(G') = (E(G) \setminus \{xy, xz\}) \cup \{yv_0, v_0v_1, v_1v_2, ..., v_{m_{22}-1}v_{m_{22}}, v_{m_{22}}z\} . \quad (7)$$

Note that the edge with endvertices u and v is denoted by uv. Note further that G' is obtained from G by replacing the path yxz by path $yv_0v_1 .... v_{m_{22}}z$.

Note that each vertex in G has degree 1, 2 or 4. Also, we have $\mu_{11}(G) = m_{11}$, $\mu_{12}(G) = m_{12}$, $\mu_{14}(G) = m_{14}$, $\mu_{24}(G) = m_{24}$, $\mu_{44}(G) = m_{44}$, so:

$$f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1. \quad (8)$$

If we have $m_{11} = 0$, $m_{12} = 0$, $m_{14} = 0$, $m_{22} \geq 3$, $m_{24} = 0$, $m_{44} = 0$, claim is trivial.

Now, let us prove the claim in the opposite direction. Suppose that:

$$f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1. \quad (9)$$

Then there is a simple connected graph G such that each vertex in G has degree 1, 2 or 4, and such that $\mu_{ij}(G) = m_{ij}$, for each $1 \leq i, j \leq 4$, $i \neq j$. We distinguish two possibilities:

Case 1. Each vertex has degree 2. In this case, we have $\mu_{11}(G) = 0$, $\mu_{12}(G) = 0$, $\mu_{14}(G) = 0$, $\mu_{24}(G) = 0$, and $\mu_{44}(G) = 0$.

Case 2. There is a vertex that does not have degree 2. Since G is connected, there is a vertex x of degree 2 that is adjacent to vertex y such that $d_G(y) \neq 2$, so $m_{12} + m_{24} > 0$. Let $p_1, ..., p_k$ be the maximal induced paths with all vertices of degree 2 (in G). Denote terminal vertices of p_i by x_i^1 and x_i^2, for each $i = 1, ..., k$. Denote by y_i^j the only element of the set $N_G(x_i^j) \setminus V(p_i)$. Let G' be the graph such that

$$V(G') = \left(V(G) \setminus \left(\bigcup_{i=1}^{k} V(p_i) \right) \right) \cup \{z_1, z_2, \ldots, z_k\}$$

$$E(G') = \left(E(G) \setminus \left(\bigcup_{i=1}^{k} E(p_i) \cup \{x_i^1 y_i^1, x_i^2 y_i^2\} \right) \right) \cup \bigcup_{i=1}^{k} \{y_i^1 z_i, y_i^2 z_i\} \quad (10)$$

Note that G' is a simple connected graph such that each vertex of G' has degree 1, 2 or 4, and $\mu_{11}(G) = m_{11}$, $\mu_{12}(G) = m_{12}$, $\mu_{14}(G) = m_{14}$, $\mu_{22}(G) = 0$, $\mu_{24}(G) = m_{24}$, and $\mu_{44}(G) = m_{44}$, so:

$$f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1 \quad (11)$$

and the claim is proven.

Lemma 3. – We have:

$$[f(0, m_{12}, m_{14}, 0, m_{24}, m_{44}) = 1] \Leftrightarrow$$

$$\Leftrightarrow \begin{bmatrix} [(m_{12} \leq 4) \wedge (f(0,0,m_{12}+m_{14},0,m_{24}-m_{12},m_{44})=1)] \vee \\ [(m_{12}=2) \wedge (m_{14}=0) \wedge (m_{24}=0) \wedge (m_{44}=0)] \end{bmatrix}. \quad (12)$$

Proof: Suppose that

$$f(0, m_{12}, m_{14}, 0, m_{24}, m_{44}) = 1 , \quad (13)$$

holds and that

$$(m_{12} = 2) \wedge (m_{14} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0) \quad (14)$$

does not hold.

Then, there is a simple connected graph G such that each vertex in G has degrees 1, 2 and 4, such that $\mu_{11}(G) = 0$, $\mu_{12}(G) = m_{12}$, $\mu_{14}(G) = m_{14}$, $\mu_{22}(G) = 0$, $\mu_{24}(G) = m_{24}$, and $\mu_{44}(G) = m_{44}$. Denote by $x_1, x_2, ..., x_{m_{12}}$ vertices of degree 1, each of which is adjacent with a vertex of degree 2 and denote by $y_1, y_2, ..., y_{m_{12}}$ vertices of degree 2, each of which is adjacent with a vertex of degree 1. Also, denote $N_G(y_i) = \{x_i, z_i\}$ for each $i = 1, ..., m_{12}$. Note that $d_G(z_i) = 4$ for each $i = 1, ..., m_{12}$.

Let graph G' be the graph such that:

$$V(G') = (V(G) \setminus \{y_1, y_2, ..., y_{m_{14}}\}$$

$$E(G') = (E(G) \setminus (\{x_1y_1, ..., x_{m_{14}}y_{m_{14}}\} \cup \{y_1z_1, ..., y_{m_{14}}z_{m_{14}}\})) \cup \{x_1y_1, ..., x_{m_{14}}y_{m_{14}}\} . \quad (15)$$

Note that G' is a simple connected graph such that each vertex G' has degree 1, 2, or 4, and $\mu_{11}(G) = 0$, $\mu_{12}(G) = 0$, $\mu_{14}(G) = m_{14} + m_{12}$, $\mu_{22}(G) = 0$, $\mu_{24}(G) = m_{24} - m_{12}$, and $\mu_{44}(G) = m_{44}$, so

$$f(0, 0, m_{14} + m_{12}, 0, m_{24} - m_{12}, m_{44}) = 1 . \quad (16)$$

Let us prove the claim in the opposite direction. If

$$(m_{12} = 2) \wedge (m_{14} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0) \quad (17)$$

holds, the claim is trivial, so suppose that $m_{12} \leq m_{14}$ and

$$f(0, 0, m_{12} + m_{14}, 0, m_{24} - m_{12}, m_{44}) = 1 . \quad (18)$$

Then there is a simple connected graph such that each vertex in G has degree 1, 2 or 4 and such that $\mu_{11}(G) = 0$, $\mu_{12}(G) = 0$, $\mu_{14}(G) = m_{14} + m_{12}$, $\mu_{22}(G) = 0$, $\mu_{24}(G) = m_{24} - m_{12}$, and $\mu_{44}(G) = m_{44}$. Let pick up arbitrary m_{12} vertices of degree 1 that are adjacent to vertices of degree 4 and denote them by $x_1, ..., x_{m_{14}}$. Also, denote $N_G(x_i) = y_i$, $i = 1, ..., m_{14}$. Let G' be a graph such that:

$$V(G') = V(G) \cup \{z_1, z_2, ..., z_{m_{14}}\}$$

$$E(G') = (E(G) \cup (\{y_1z_1, ..., y_{m_{14}}z_{m_{14}}\} \cup \{x_1z_1, ..., x_{m_{14}}z_{m_{14}}\}) \setminus \{x_1y_1, ..., x_{m_{14}}y_{m_{14}}\} . \quad (19)$$

Note that G' is a simple connected graph such that each vertex of G' has degree 1, 2 or 4, and $\mu_{11}(G') = 0$, $\mu_{12}(G') = m_{12}$, $\mu_{14}(G') = m_{14}$, $\mu_{22}(G') = 0$, $\mu_{24}(G') = m_{24}$, and $\mu_{44}(G') = m_{44}$, so:

$$f(0,\ m_{12},\ m_{14},\ 0,\ m_{24} - m_{12},\ m_{44}) = 1\ . \qquad (20)$$

Lemma 4. – Let $k \geq 2$ and let $p_1,..., p_k \in \{0,1,2,3,4\}$, such that $p_1 \leq p_2 \leq ... p_k$. Let $q \in \mathcal{N}$ such that $2q \leq \sum_{i=1}^{k}(4-p_i)$. If $p_1 - p_2 \leq 1$, then there are numbers $i_1, i_2,..., i_q, j_1, j_2,..., j_q \in \{1,..., k\}$, such that $i_l \neq j_l$, $l = 1,...,q$, and

$$p_i + \text{card}\{l_0 : 1 \leq l_0 \leq q,\ i_{l_0} = i\} + \text{card}\{l_0 : 1 \leq l_0 \leq q,\ j_{l_0} = i\} \leq 4,\ 1 \leq i \leq k\ . \qquad (21)$$

Note that card X stands for the number of elements in set X.

Proof: We prove the claim by induction on q. Suppose that $q = 1$. Note that $p_1, p_2 \leq 3$, so it is sufficient to take $i_1 = 1$ and $j_1 = 2$. Now, suppose that the claim holds for q and let us prove it for $q + 1$ Take $i_{q+1} = 1$ and $j_{q+1} = 2$. Denote $p_1' = p_1 - 1$, $p_2' = p_2 - 1$ and $p_i' = p_i$ for each $3 \leq i \leq k$. Denote by $p_1'',..., p_k''$ numbers $p_1',..., p_k'$ sorted in the ascending order. More formally, collections $\{p_1', p_2',..., p_k'\}$ and $\{p_1'', p_2'',..., p_k''\}$ are equal and $p_1'' \leq p_2'' \leq ... \leq p_k''$. Denote by ϕ a bijection such that

$$p_k' = p_{\phi(k)}''. \qquad (22)$$

Note that $p_1'' - p_2'' \leq 1$. So, by the inductive hypothesis, there are numbers $i_1', i_2',..., i_q', j_1', j_2',..., j_q' \in \{1,..., k\}$ such that $i_l' \neq j_l'$, $l = 1,...,$ k, and

$$p_i'' + \text{card}\{l_0' : 1 \leq l_0 \leq q,\ i_{l_0}' = i\} + \text{card}\{j_0' : 1 \leq l_0 \leq q,\ j_{l_0}' = i\} \leq 4,\ 1 \leq l \leq k\ . \qquad (23)$$

So, it is sufficient to take numbers

$$i_l = \phi(i_l'),\ 1 \leq l \leq q \qquad (24)$$

$$j_l = \phi(j_l'),\ 1 \leq l \leq q \qquad (25)$$

and i_{q+1} and j_{q+1}.

Lemma 5. – We have

$$[f(0,\ 0,\ m_{14},\ 0,\ m_{24},\ m_{44}) = 1] \Leftrightarrow$$

$$\Leftrightarrow \left\{ \begin{array}{l} \left[\begin{array}{l} (n_4 \in \mathcal{N}) \wedge \left(\frac{m_{24}}{2} \in \mathcal{N} \right) \wedge \\ \left(n_4 - 1 - \frac{n_{24}}{2} \leq m_{44} \leq \binom{n_4}{2} \right) \wedge (n_4 \geq 2) \end{array} \right] \vee \\ [(n_4 = 1) \wedge (m_{14} = 4)] \end{array} \right\} \qquad (26)$$

where $n_4 = \frac{1}{4}(m_{14} + m_{24} + 2m_{44})$.

Proof: First, let us prove

$$\left\{ \begin{array}{l} \left[\begin{array}{l} (n_4 \in \mathcal{N}) \wedge \left(\frac{m_{24}}{2} \in \mathcal{N} \right) \wedge \\ \left(n_4 - 1 - \frac{n_{24}}{2} \leq m_{44} \leq \binom{n_4}{2} \right) \wedge (n_4 \geq 2) \end{array} \right] \vee \\ [(n_4 = 1) \wedge (m_{14} = 4)] \end{array} \right\} \Rightarrow$$

$$\Rightarrow [f(0,\ 0,\ m_{14},\ 0,\ m_{24},\ m_{44}) = 1]\ . \qquad (27)$$

If $n_4 = 1$ and $m_{14} = 4$, the claim is trivial, so it remains to prove

$$\left\{ \begin{array}{l} (n_4 \in \mathcal{N}) \wedge \left(\frac{m_{24}}{2} \in \mathcal{N} \right) \wedge \\ \left(n_4 - 1 - \frac{n_{24}}{2} \leq m_{44} \leq \binom{n_4}{2} \right) \wedge (n_4 \geq 2) \end{array} \right\} \Rightarrow$$

$$\Rightarrow [f(0,\ 0,\ m_{14},\ 0,\ m_{24},\ m_{44}) = 1]\ . \qquad (28)$$

It follows from the previous Lemma that it is sufficient to construct graph G_0 with n_4 vertices and m_{44} edges such that its maximal degree $\Delta(G_0)$ is less or equal to 4 and that there are vertices x and y such that the minimal degree $\delta(G_0)$ equals $d_{G_0}(x)$ and $d_{G_0}(y) - d_{G_0}(x) \leq 1$.

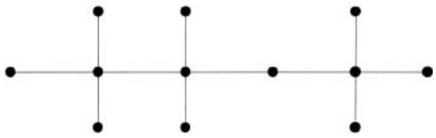
If $n_4 = 2$, the claim is trivial, so suppose that $n_4 > 2$. Denote vertices of G_0 by $x, y, z_1, z_2,..., z_{n_4-2}$. Distinguish two cases:

Case 1: $m_{44} \geq n_4 - 1$

Let $E(G_0) \supseteq \{ xz_1, z_1z_2,...,z_{n_4-3}z_{n_4-2}, z_{n_4-2}y\}$. Since $m_{44} \geq n_4 - 1$, G_0 can consist of these edges. If $m_{44} \leq \binom{n_4-2}{2} + 2$, then form arbitrary $m_{44} - (n_4 - 1)$ edges between vertices $z_1, z_2,..., z_{n_4-2}$ and we are done. Otherwise, let G_0 $[z_1, z_2,..., z_{n_4-2}]$ be a complete graph. Add $\left\lfloor \frac{m_{44} - \left(\binom{n_4-2}{2} + 2 \right)}{2} \right\rfloor$ vertices of the form xz_i and $\left\lceil \frac{m_{44} - \left(\binom{n_4-2}{2} + 2 \right)}{2} \right\rceil$ vertices of the form yz_i and the claim is proven in this case. Note that $\lfloor x \rfloor$ and $\lceil x \rceil$ stand for lower and upper integer parts of x, respectively.

Case 2: $m_{44} \leq n_4 - 1$

By using the construction of the previous case, we can construct graph G_0' such that $\mu_{11}(G_0') = 0$, $\mu_{12}(G_0') = 0$, $\mu_{14}(G_0') = m_{14}$, $\mu_{22}(G_0') = 0$, $\mu_{24}(G_0') = m_{24} - 2(n_4 - 1 - m_{44})$. Let us take $n_4 - 1 - m_{44}$ edges that connect vertices of degree 4 and replace each of them by the path of length 2. This proves Case 2. Let us illustrate this for the case $m_{14} = 8$, $m_{24} = 2$ and $m_{44} = 1$.



Let us prove the claim in the opposite direction. Suppose that:

$$f(0,\ 0,\ m_{14},\ 0,\ m_{24},\ m_{44}) = 1\ . \qquad (29)$$

Then there is a simple connected graph G such that each vertex in G has degree 1, 2 or 4 and such that $\mu_{11}(\mathrm{G}) = 0$, $\mu_{12}(\mathrm{G}) = 0$, $\mu_{14}(\mathrm{G}) = m_{14}$, $\mu_{22}(\mathrm{G}) = 0$, $\mu_{24}(\mathrm{G}) = m_{24}$ and $\mu_{44}(\mathrm{G}) = m_{44}$. If there is only one vertex of degree 4 in G, it can be easily checked that $m_{14} = 4$, $m_{24} = 0$, and that $m_{44} = 4$ or equivalently $n_4 = 4$ and $m_{14} = 4$.

Thus, it remains to prove the claim when there are at least two vertices of degree 4 in G. Note that the number of vertices of degree 4 in G is:

$$(m_{14} + m_{24} + 2m_{44})\ /\ 4 = n_4\ . \qquad (30)$$

So, indeed $n_4 \in \mathbb{N}$ and $n_4 \geq 2$. Also, note that the number of vertices of degree 2 in G is $m_{24} / 2$ and so this has to be a natural number or zero.

Since G is connected, it follows that:

$$n_4 - 1 - m_{24}\ /\ 2 \leq m_{44}, \qquad (31)$$

and since G is simple, it follows that

$$m_{44} \leq \binom{n_4}{2}. \qquad (32)$$

Thus, the Lemma is proven.

By combining the results of Lemmas 1–5, one obtains:

$$\{f(m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1\}$$

$$\Leftrightarrow \left\{\begin{array}{l} [(m_{11} = 1) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ [(m_{11} = 0) \wedge (f(0, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}) = 1)] \end{array}\right\}$$

$$\Leftrightarrow \left\{\begin{array}{l} [(m_{11} = 1) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ [(m_{11} = 0) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} \geq 3) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ \{[(m_{11} = 0) \wedge [(m_{22} = 0) \vee [(m_{12} + m_{24} > 0)]] \wedge f(0, m_{12}, m_{14}, 0, m_{24}, m_{44}) = 1]\} \end{array}\right\}$$

$$\Leftrightarrow \left\{\begin{array}{l} [(m_{11} = 1) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ [(m_{11} = 0) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} \geq 3) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ \{[(m_{11} = 0) \wedge [(m_{22} = 0) \vee [(m_{12} + m_{24} > 0)]] \wedge f(0, m_{12}, m_{14}, 0, m_{24}, m_{44}) = 1]\} \end{array}\right\}$$

$$\Leftrightarrow \left\{\begin{array}{l} [(m_{11} = 1) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ [(m_{11} = 0) \wedge (m_{12} = 0) \wedge (m_{14} = 0) \wedge (m_{22} \geq 3) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ [(m_{11} = 0) \wedge (m_{12} = 2) \wedge (m_{14} = 0) \wedge (m_{24} = 0) \wedge (m_{44} = 0)] \vee \\ \left\{\left\{\begin{array}{l} (m_{11} = 0) \wedge [(m_{22} = 0) \vee [(m_{12} + m_{24} > 0)]] \wedge (m_{12} \leq m_{24}) \wedge \\ \left\{\begin{array}{l} [(m_{14} + m_{12} = 4) \wedge (m_{24} - m_{12} = 0) \wedge (m_{44} = 0)] \vee \\ \left[\begin{array}{l} \left(\dfrac{m_{14} + m_{24} + 2m_{44}}{4} \in N\right) \wedge \left(\dfrac{m_{24} - m_{12}}{2} \in N_0\right) \wedge \\ \left(\dfrac{m_{14} + m_{24} + 2m_{44}}{4} - 1 - \dfrac{m_{24} - m_{12}}{2} \leq m_{44} \leq \left(\begin{array}{c} \dfrac{m_{14} + m_{24} + 2m_{44}}{4} \\ 2 \end{array}\right)\right) \\ \wedge \left(\dfrac{m_{14} + m_{24} + 2m_{44}}{4} \geq 2\right) \end{array}\right] \end{array}\right\} \end{array}\right\}\right\} \end{array}\right\}$$

(cont.)

(cont.)

$$
\Leftrightarrow \left\{
\begin{array}{l}
\left[(m_{11}=1)\wedge(m_{12}=0)\wedge(m_{14}=0)\wedge(m_{22}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee\\
\left[(m_{11}=0)\wedge(m_{12}=0)\wedge(m_{14}=0)\wedge(m_{22}\geq 3)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee\\
\left[(m_{11}=0)\wedge(m_{12}=2)\wedge(m_{14}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee\\
\left\{\left\{\begin{array}{l}
\left\{\begin{array}{l}(m_{11}=0)\wedge\left[(m_{22}=0)\vee\left[(m_{12}+m_{24}>0)\right]\right]\wedge(m_{12}\leq m_{24})\wedge\\
(m_{14}+m_{12}=4)\wedge(m_{24}-m_{12}=0)\wedge(m_{44}=0)\end{array}\right\}\vee\\
\left\{\begin{array}{l}(m_{11}=0)\wedge\left[(m_{22}=0)\vee\left[(m_{12}+m_{24}>0)\right]\right]\wedge(m_{12}\leq m_{24})\wedge\\
\left[\begin{array}{l}\left(\frac{m_{14}+m_{24}+2m_{44}}{4}\in N\right)\wedge\left(\frac{m_{24}-m_{12}}{2}\in N_0\right)\wedge\\
\left(\frac{m_{14}+m_{24}+2m_{44}}{4}-1-\frac{m_{24}-m_{12}}{2}\leq m_{44}\leq\left(\frac{\frac{m_{14}+m_{24}+2m_{44}}{4}}{2}\right)\right)\\
\wedge\left(\frac{m_{14}+m_{24}+2m_{44}}{4}\geq 2\right)\end{array}\right]\end{array}\right\}
\end{array}\right\}\right\}
\end{array}\right\}
$$

$$
\Leftrightarrow \left\{
\begin{array}{l}
\left[(m_{11}=1)\wedge(m_{12}=0)\wedge(m_{14}=0)\wedge(m_{22}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee\\
\left[(m_{11}=0)\wedge(m_{12}=0)\wedge(m_{14}=0)\wedge(m_{22}\geq 3)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee\\
\left[(m_{11}=0)\wedge(m_{12}=2)\wedge(m_{14}=0)\wedge(m_{24}=0)\wedge(m_{44}=0)\right]\vee\\
\left\{\left\{\begin{array}{l}
\left\{(m_{11}=0)\wedge\left[(m_{22}=0)\vee(m_{12}>0)\right]\wedge(m_{14}+m_{12}=4)\wedge(m_{12}=m_{24})\wedge(m_{44}=0)\right\}\vee\\
\left\{\begin{array}{l}(m_{11}=0)\wedge\left[(m_{22}=0)\vee\left[(m_{12}+m_{24}>0)\right]\right]\wedge(m_{12}\leq m_{24})\wedge\\
\left[\begin{array}{l}\left(\frac{m_{14}+m_{24}+2m_{44}}{4}\in N\right)\wedge\left(\frac{m_{24}-m_{12}}{2}\in N_0\right)\wedge\\
\left(\frac{m_{14}+m_{24}+2m_{44}}{4}-1-\frac{m_{24}-m_{12}}{2}\leq m_{44}\leq\left(\frac{\frac{m_{14}+m_{24}+2m_{44}}{4}}{2}\right)\right)\\
\wedge\left(\frac{m_{14}+m_{24}+2m_{44}}{4}\geq 2\right)\end{array}\right]\end{array}\right\}
\end{array}\right\}\right\}
\end{array}\right\}
\quad (33)
$$

and this finally proves Theorem 1.

CONCLUSIONS

The difficult problem of determining whether there are graph(s) with a prescribed m_{ij} sequence, where m_{ij} denotes how many edges connect vertices of degree i with vertices of degree j, is tackled in this paper. We have been able to solve the problem for the case of graphs with degrees 1, 2 and 4 and the findings are given by Theorem 1, which gives the necessary and sufficient conditions for the existence of graph(s) with the prescribed sequence m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}. Although there is a multitude of chemical moieties covered by our special consideration, it will be of the outmost importance for chemistry to allow also vertices of degree 3, *i.e.*, to consider the existence of molecular graph(s) with prescribed sequences of m_{ij}'s, i, j = 1, 2, 3, 4.

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SAŽETAK

O molekularnim grafovima valencije 1, 2 i 4 sa zadanim brojevima veza

Damir Vukičević i Ante Graovac

U radu su dani nužni i dovoljni uvjeti za egzistenciju molekularnoga grafa(ova) sa zadanim slijedom m_{11}, m_{12}, m_{14}, m_{22}, m_{24}, m_{44}, gdje m_{ij} označava broj bridova (veza) što povezuju vrhove (atome) stupnjeva i i j. Osnovni rezultat iskazan je Teoremom 1 koji je primjenljiv na vrlo široku klasu molekula sa valencijama 1, 2 i 4.