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Thorny graphs. I. Valence connectivities

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Abstract

Monocyclic graphs (*i.e.*, connected graphs with a unique cycle) whose every vertex has degree at most 4 model many chemical compounds of practical interest. Therefore, it is of interest to create specialized software for the analyses of such graphs. In order to develop such software a large number of efficient algorithms have to be developed. These algorithms (in order to be really efficient) have to rely on mathematical theory. Here we give several theorems that are incorporated in the software *Thorny Graph Calculator*. Algorithms based on these theorems are able to almost instantly solve the problems for graphs up to a few hundred vertices.

With $\mu_{ij}(G)$, we denote the number of edges in a graph G that connect vertices of degrees i and j. The contribution of this paper to the algorithms of the software *Thoryn Graph Calculator* is the following: we give necessary and sufficient conditions on numbers $\mu_{ij}(G)$ such that graph with prescribed thorns exists.

Since, numbers $\mu_{ij}(G)$ are incorporated in many topological indices (let us just mention the Randić index and the Zagreb indices), these results may be of use to those interested, for example, in QSAR and QSPR modeling.

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1. Introduction

Thorny graph is a graph that can be obtained from a parent connected graph by attaching new vertices of valence one to each vertex of the parent graph. In the present report we adopted term *thorny graphs* after Bytautas *et al*. [1], but these autors have also used the term *thorn graphs* [2]. The protype of a thorny graph is a plerogram of Cayley [3]. Plerograms are molecular graphs in which all atoms are represented by vertices, the so called hydrogen-filled (molecular) graphs. Cayley called the hydrogen-deleted graphs kenograms. Plerograms and kenograms have been used in various contexts in recent years [1,2,4-6]. Since plerograms and kenograms are not diagrams but graphs, we named them plerographs and kenographs [7]. Several classes of thorny graphs, such as thorny trees, thorny rings, thorny rods, thorny stars, have been studied in recent years [1,2]. Thorny graphs found use in theory of polymers [8,9], especially for dendrimers [10,11].

In extension of the above metioned papers, we report in three related papers some of mathematical and computational properties of thorny graphs. The standard graph-theoretical apparatus will be used [12-14].

The results obtained in this paper require a lot of tedious mathematical calculations. Here, we do not incorporate the proofs of the presented theorems. Instead are made available on internet in a paper of about 35 pages (http://www.pmfst.hr/~vukicevi/ProjEngIndex.htm). On the same address the pseudo-code of the algorithm will also be presented together with its software and the manual (for the free download).

2. Mathematical aspects

Let G be any graph with maximal degree at most 4. Denote by $\mu_{ij}(G)$, $1 \le i \le j \le 4$, number of edges that connect vertices of degrees i and j in G (this edges are also termed as ij-valence connectivities). Also denote $\mu(G) = \begin{pmatrix} \mu_{11}(G), \mu_{12}(G), \mu_{13}(G), \mu_{14}(G), \mu_{22}(G), \\ \mu_{23}(G), \mu_{24}(G), \mu_{33}(G), \mu_{34}(G), \mu_{44}(G) \end{pmatrix}$. If an edge connect vertices of degrees i and j, we say that edge is of type e_{ij}.

Let $\alpha : \{0,1\}^8 \times N_0^{10} \to \{0,1\}$ be the function defined by

$\alpha\begin{pmatrix} i_1, i_2, i_3, i_4, i_5, i_6, i_7, i_8, m_{11}, m_{12}, m_{13}, \\ m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix} = 1$ if and only if there is a thorny cycle G such that

$\mu(G) = \begin{pmatrix} m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix}$ with the following thorn allowed: methyl-thorn (if $i_1 = 1$);

ethyl-thorn (if $i_2 = 1$); propyl-thorn (if $i_3 = 1$); isopropyl-thorn (if $i_4 = 1$); butyl-thorn (if $i_5 = 1$); (2-methyl-propyl)-thorn (if $i_6 = 1$); (1-methyl-propyl)-thorn (if $i_7 = 1$); and (1,1-dimethyl-ethyl)-thorn (if $i_8 = 1$).

Let $\beta : \{0,1\}^3 \times \{0,1,2\} \times \{0,1\}^3 \times N_0^{11} \to \{0,1\}$ be the function defined by $\beta\begin{pmatrix} i_1, i_2, i_3, i_4, i_5, i_6, i_8, m_{11}, m_{12}, m_{13}, \\ m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r \end{pmatrix} = 1$ if and only if "There is a thorny cycle G such that $\mu(G) = \begin{pmatrix} m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix}$ with the following thorn allowed: methyl-thorn (if $i_1 = 1$); ethyl-thorn (if $i_2 = 1$); propyl-thorn (if $i_3 = 1$); isopropyl-thorn (if $i_4 > 0$); butyl-thorn (if $i_5 = 1$); (2-methyl-propyl)-thorn (if $i_6 = 1$); (1,1-dimethyl-ethyl)-thorn (if $i_8 = 1$); and such that there are exactly r isopropyl-thorns (if $i_4 = 2$) or there are at least r isopropyl-thorns (if $i_4 < 2$). First, we give the theorem that determines the value of the function α in terms of the function β :

Theorem 1 $\alpha\begin{pmatrix} i_1, i_2, i_3, i_4, i_5, i_6, i_7, i_8, m_{11}, m_{12}, m_{13}, \\ m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix} = 1$ if and only if one of the following statements holds:

1) $(i_7 = 0)$ and $\beta\begin{pmatrix} i_1, i_2, i_3, i_4, i_5, i_6, i_8, m_{11}, m_{12}, m_{13}, \\ m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, 0 \end{pmatrix} = 1$.

2) $(i_7 \neq 0)$ and $(i_4 = 0)$ and

$$\left(\exists i \in \{0,1,\ldots,\min\{m_{12}, m_{13}, m_{23}\}\}\right)\beta\begin{pmatrix} i_1, i_2, i_3, 2, i_5, i_6, i_8, m_{11}, m_{12} - i, m_{13} + i, \\ m_{14}, m_{22}, m_{23} - i, m_{24}, m_{33}, m_{34}, m_{44}, i \end{pmatrix} = 1$$

3) $(i_7 \neq 0)$ and $(i_4 \neq 0)$ and

$$\left(\exists i \in \{0,1,\ldots,\min\{m_{12}, m_{13}, m_{23}\}\}\right)\beta\begin{pmatrix} i_1, i_2, i_3, i_4, i_5, i_6, i_8, m_{11}, m_{12} - i, m_{13} + i, \\ m_{14}, m_{22}, m_{23} - i, m_{24}, m_{33}, m_{34}, m_{44}, i \end{pmatrix} = 1. \blacksquare$$

Let function $\gamma : \{0,1\}^2 \times \{0,1,2\} \times \{0,1\}^2 \times N_0^{11} \to \{0,1\}$ be given by $\gamma\begin{pmatrix} j_2, i_1, i_4, i_6, i_8, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r \end{pmatrix} = 1$ if and only if "There is a thorny cycle G such that $\mu(G) = \begin{pmatrix} m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix}$ with the following thorn allowed: methyl-thorn (if $i_1 = 1$); ethyl-thorn (if $j_2 = 1$); isopropyl-thorn (if $i_4 > 1$); (2-methyl-propyl)-thorn (if $i_6 = 1$); (2-methyl-propyl)-thorn (if $i_7 = 1$); and (1,1-dimethyl-ethyl)-thorn (if $i_8 = 1$) and there are at least r isopropyl-thorns (if $i_4 \neq 2$) or there are exactly r isopropyl-thorns (if $i_4 = 2$). The next theorem theorem determines the value of the function β in terms of the function γ :

Theorem 2 $\beta\begin{pmatrix} i_1,i_2,i_3,i_4,i_5,i_6,i_8,m_{11},m_{12},m_{13}, \\ m_{14},m_{22},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1$ if and only if one of the following statements hold:

1) $(i_3=0)$ and $(i_5=0)$ and $\left(\gamma\begin{pmatrix} i_2,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

2) $(i_2=0)$ and $(i_3=1)$ and $(i_5=0)$ and $(m_{22}\ge m_{12})$ and $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22}-m_{12},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

3) $(i_2=1)$ and $(i_3=1)$ and $(i_5=0)$ and one of the following holds:

3.1) $(m_{12}\ge m_{22})$ and $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ 0,m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

3.2) $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

4) $(i_2=0)$ and $(i_3=0)$ and $(i_5=1)$ and $(m_{22}\ge 2\cdot m_{12})$ and $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22}-2\cdot m_{12},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

5) $(i_2=1)$ and $(i_3=0)$ and $(i_5=1)$ and one of the following holds:

5.1) $(2\cdot m_{12}\ge m_{22})$ and $(m_{22}=0(\text{mod}\,2))$ and $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ 0,m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

5.2) $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22}-m_{12},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

6) $(i_2=0)$ and $(i_3=1)$ and $(i_5=1)$ and $(m_{22}\ge m_{12})$ and one of the following holds:

6.1) $(2\cdot m_{12}\ge m_{22})$ and $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ 0,m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

6.2) $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22}-m_{12},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

7) $(i_2=1)$ and $(i_3=1)$ and $(i_5=1)$ and one of the following holds:

7.1) $(2\cdot m_{12}\ge m_{22})$ and $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ 0,m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$

7.2) $\left(\gamma\begin{pmatrix} 1,i_1,i_4,i_6,i_8,m_{11},m_{12},m_{13},m_{14}, \\ m_{22},m_{23},m_{24},m_{33},m_{34},m_{44},r \end{pmatrix}=1\right)$ ■

Let function $\delta:\{0,1\}^2\times\{0,1,2\}\times\{0,1\}\times N_0^{12}\to\{0,1\}$ be given by

$\delta\begin{pmatrix} j_1,j_2,j_3,j_4,m_{11},m_{12},m_{13},m_{14}, \\ m_{22},m_{23},m_{24},m_{33},m_{34},m_{44},r,s \end{pmatrix}=1$ if and only if "There is a thorny cycle G such that

$\mu(G)=\begin{pmatrix} m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix}$ with the following thorn allowed: methyl-thorn (if $j_1 = 1$); ethyl-thorn (if $j_2 = 1$); isopropyl-thorn (if $j_3 > 1$); and (1,1-dimethyl-ethyl)-thorn (if $j_4 = 1$) there are at least r isopropyl-thorns (if $i_4 \neq 2$) or there are exactly r isopropyl-thorns (if $i_4 = 2$); and there are at least s ethyl-thorns. The following theorem determines the value of the function γ in terms of the function δ :

Theorem 3 $\gamma\begin{pmatrix} j_2, i_1, i_4, i_6, i_8, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s \end{pmatrix} = 1$ if and only if one of the following holds:

1) $(i_6 = 0)$ and $\delta\begin{pmatrix} i_1, j_2, i_4, i_8, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, 0 \end{pmatrix} = 1$

2) $(i_6 = 1)$ and $((j_2 = 1)$ or $(m_{12} = 0))$ and

$$\left(\exists i = 0,\dots,\min\left\{\left\lfloor \frac{m_{13}-2r}{2} \right\rfloor, m_{23}\right\}\right)\left(\delta\begin{pmatrix} i_1, 1, i_4, i_8, m_{11}, m_{12}+i, m_{13}-2\cdot i, m_{14}, \\ m_{22}, m_{23}-i, m_{24}, m_{33}, m_{34}, m_{44}, r, i \end{pmatrix} = 1\right) \blacksquare$$

Let function $\varepsilon : \{0,1\}^2 \times \{0,1,2\} \times \{0,1\} \times N_0^{16} \to \{0,1\}$ be given by $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, x, y, z, u \end{pmatrix} = 1$ if and only if "There is a thorny cycle G such that $\mu(G)=\begin{pmatrix} m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \end{pmatrix}$ with the following thorn allowed: methyl-thorn (if $j_1 = 1$); ethyl-thorn (if $j_2 = 1$); isopropyl-thorn (if $j_3 > 1$); and (1,1-dimethyl-ethyl)-thorn (if $j_4 = 1$) there are at least r isopropyl-thorns (if $i_4 \neq 2$) or there are exactly r isopropyl-thorns (if $i_4 = 2$); there are at least s ethyl-thorns; there are u ethyl-thorns adjacent to vertices of degree 3; x isopropyl-thorns adjacent with vertices of degree 3; y isopropyl-thorns adjacent to vertices of degree 4; z (1,1-dimethyl-ethyl)-thorns adjacent with vertices of degree 4; and there are n_3 vertices of degree 3. The value of the function δ can be expressed in terms of the function ε by:

Theorem 4. $\delta\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s \end{pmatrix} = 1$ if and only if $m_{12} \geq s$; $m_{11} = 0$; $n_3, n_4 \in N$; $n_1 = 2n_4 + n_3$ and one of the following claims hold:

1) $m_{34} - n_3 + m_{13} + m_{23} = 0 (\bmod 2)$ and $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, \\ m_{33}, (m_{34} - n_3 + m_{13} + m_{23})/2, m_{44}, m_{23} \end{pmatrix} = 1$

2) $j_1 = 1$ and one of the following claims hold

2.1) $m_{34} - n_3 + m_{13} + m_{23} = 0(\mathrm{mod}\,2)$ and $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, \\ m_{33}, (m_{34} - n_3 + m_{13} + m_{23})/2, 0, m_{23} \end{pmatrix} = 1$

2.2) $m_{34} - n_3 + m_{13} + m_{12} - m_{24} = 0(\mathrm{mod}\,2)$ and one of the following claims hold

2.2.1) $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, \\ 0, (m_{34} - n_3 + m_{13} + m_{12} - m_{24})/2, m_{44}, m_{12} - m_{24} \end{pmatrix} = 1$

2.2.2) $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, r - (m_{34} - n_3 + m_{13} + m_{12} - m_{24})/2, \\ (m_{34} - n_3 + m_{13} + m_{12} - m_{24})/2, m_{44}, m_{12} - m_{24} \end{pmatrix} = 1$

3) $j_1 = 0$ and one of the following claims hold

3.1) $m_{34} - n_3 + m_{13} + m_{23} = 0(\mathrm{mod}\,2)$ and $m_{14} = 0(\mathrm{mod}\,3)$ and

$\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, m_{33}, (m_{34} - n_3 + m_{13} + m_{23})/2, \\ m_{14}/3 - n_3 + m_{13} - (m_{34} - n_3 + m_{13} + m_{23})/2 + m_{23}, m_{23} \end{pmatrix} = 1$

3.2) $m_{34} - n_3 + m_{13} + m_{12} - m_{24} + m_{23} = 0(\mathrm{mod}\,2)$ and $m_{13} = 0(\mathrm{mod}\,2)$ and

$\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, m_{13}/2 - (m_{34} - n_3 + m_{13} + m_{12} - m_{24} + m_{23})/2, \\ (m_{34} - n_3 + m_{13} + m_{12} - m_{24} + m_{23})/2, m_{44}, m_{12} - m_{24} \end{pmatrix} = 1$

4) The following holds:

4.1) $m_{24} - m_{12} + m_{34} - n_3 + m_{13}$ is an even number

4.2) $(m_{22} = 0)$ or $(m_{23} + m_{24} - m_{12} = 0)$

4.3) There are integers x, y, z, u such that:

4.3.1) $x + y \ge r$

4.3.2) $x \ge 0$

4.3.3) $y \ge 0$

4.3.4) $z \ge 0$

4.3.5) $u \ge 0$

4.3.6) $m_{13} - 2x - 2y \ge 0$

4.3.7) $n_3 - m_{13} + y - u \ge 0$

4.3.8) $m_{14} - 3n_3 + 3m_{13} - 3y + 3u - 3z \ge 0$

4.3.9) $m_{12} - u \ge 0$

4.3.10) $x + y = r$ or $j_3 < 2$

4.3.11) $m_{13} - 2x - 2y = 0$ or $j_1 > 0$

4.3.12) $m_{14} - 3n_3 + 3m_{13} - 3y + 3u - 3z = 0$ or $j_1 > 0$

4.3.13) $u = 0$ or $j_2 > 0$

4.3.14) $m_{12} - u = 0$ or $j_2 > 0$

4.3.15) $x = 0$ or $j_3 > 0$

4.3.16) $y = 0$ or $j_3 > 0$
4.3.17) $n_3 - m_{13} + y - u = 0$ or $j_4 > 0$
4.3.18) $z = 0$ or $j_4 > 0$
4.3.19) $m_{22} + m_{23} + m_{24} + m_{33} + m_{34} - m_{12} - n_3 + m_{13} - 3 + u - x - 2y - z \geq 0$
4.3.20) $m_{23} + m_{34} - n_3 + m_{13} - 2 - 2y \geq 0$
4.3.21) $m_{24} - m_{12} + m_{34} - n_3 + m_{13} - 2 + 2u - 2y \geq 0$
4.3.22) $m_{23} - u \geq 0$
4.3.23) $m_{24} - m_{12} + u \geq 0$
4.3.24) $m_{33} - x \geq 0$
4.3.25) $m_{34} - n_3 + m_{13} - 2y + u \geq 0$
4.3.26) $m_{44} - z \geq 0$

where

$n_1 = m_{12} + m_{13} + m_{14}$; $n_3 = \dfrac{m_{13} + m_{23} + 2m_{33} + m_{34}}{3}$ and $n_4 = \dfrac{m_{14} + m_{24} + m_{34} + 2m_{44}}{4}$.■

Let function $\zeta : \{0,1\}^2 \times \{0,1,2\} \times \{0,1\} \times N_0^{12} \to \{0,1\}$ be given by $\zeta\begin{pmatrix} j_1, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s \end{pmatrix} = 1$ if and only if they satisfy the condition 4) of the last Lemma. Now, we can reformulate the last Theorem as:

Theorem 5. $\delta\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s \end{pmatrix} = 1$ if and only if $m_{12} \geq s$; $m_{11} = 0$; $n_3, n_4 \in N$ and one of the following claims hold:

1) $m_{34} - n_3 + m_{13} + m_{23} = 0 \pmod 2$ and $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, \\ m_{33}, (m_{34} - n_3 + m_{13} + m_{23})/2, m_{44}, m_{23} \end{pmatrix} = 1$

2) $j_1 = 1$ and one of the following claims hold

2.1) $m_{34} - n_3 + m_{13} + m_{23} = 0 \pmod 2$ and $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, \\ m_{33}, (m_{34} - n_3 + m_{13} + m_{23})/2, 0, m_{23} \end{pmatrix} = 1$

2.2) $m_{34} - n_3 + m_{13} + m_{12} - m_{24} = 0 \pmod 2$ and one of the following claims hold

2.2.1) $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, \\ 0, (m_{34} - n_3 + m_{13} + m_{12} - m_{24})/2, m_{44}, m_{12} - m_{24} \end{pmatrix} = 1$

2.2.2) $\varepsilon\begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, r - (m_{34} - n_3 + m_{13} + m_{12} - m_{24})/2, \\ (m_{34} - n_3 + m_{13} + m_{12} - m_{24})/2, m_{44}, m_{12} - m_{24} \end{pmatrix} = 1$

3) $j_1 = 0$ and one of the following claims hold

3.1) $m_{34} - n_3 + m_{13} + m_{23} = 0 \pmod 2$ and $m_{14} = 0 \pmod 3$ and

$$\varepsilon \begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, m_{33}, (m_{34} - n_3 + m_{13} + m_{23})/2, \\ m_{14}/3 - n_3 + m_{13} - (m_{34} - n_3 + m_{13} + m_{23})/2 + m_{23}, m_{23} \end{pmatrix} = 1$$

3.2) $m_{34} - n_3 + m_{13} + m_{12} - m_{24} + m_{23} = 0 \pmod 2$ and $m_{13} = 0 \pmod 2$ and

$$\varepsilon \begin{pmatrix} j_2, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, \\ m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s, m_{13}/2 - (m_{34} - n_3 + m_{13} + m_{12} - m_{24} + m_{23})/2, \\ (m_{34} - n_3 + m_{13} + m_{12} - m_{24} + m_{23})/2, m_{44}, m_{12} - m_{24} \end{pmatrix} = 1$$

4) $\zeta \begin{pmatrix} j_1, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s \end{pmatrix} = 1$ ■

Finally, we show that:

Theorem 6 $\zeta \begin{pmatrix} j_1, j_2, j_3, j_4, m_{11}, m_{12}, m_{13}, m_{14}, \\ m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}, r, s \end{pmatrix} = 1$ if and only if

1) $m_{24} - m_{12} + m_{34} - n_3 + m_{13}$ is an even number
2) $(m_{22} = 0)$ or $(m_{23} + m_{24} - m_{12} > 0)$
3) $(b = 0 \pmod 3)$ or $j_1 > 0$
4) $m_{13} = 0 \pmod 2$ or $j_1 > 0$
5) $k \le j$ or $j_1 > 0$
6) $r \le k$
7) $m_{12} = 0$ or $j_2 > 0$
8) $a = -h$ or $j_1 > 0$ or $j_4 > 0$
9) $0 \ge r$ or $j_3 > 0$
10 $k = 0$ or $j_1 > 0$ or $j_3 > 0$
11) $k = r$ or $j_1 > 0$ or $j_3 \ne 2$
12) $fa \le fee$
13) $ff \le a$
14) $ff \le i$ or $j_1 > 0$
15) $0 \le fee$ or $j_2 > 0$
16) $0 \ge fa$ or $j_2 > 0$
17) $a \le i$ or $j_1 > 0$ or $j_4 > 0$
18) There is an integer y such that

18.1) $y \ge fk$
18.2) $y \le fl$
18.3) $y = 0$ or $j_3 > 0$
18.4) $y \le r$ or $j_3 \ne 2$
18.5) $y \le fh$ or $j_1 > 0$

18.6) $y \geq fg$ or $j_1 > 0$
18.7) $y \geq o$ or $j_1 > 0$
18.8) $y \geq -a$ or $j_2 > 0$
18.9) $y \leq fi$ or $j_2 > 0$
18.10) $y \leq fj$ or $j_4 > 0$
18.11) $y \geq -i$ or $j_1 > 0$
18.12) $y = -a$ or $j_2 > 0$ or $j_4 > 0$ ■

3. Computational aspects

Using the above theorems, we can make an efficient algorithm that solves our problem. An algorithm consists of 7 functions: TestA (which calculates function α), TestB (which calculates function β), TestC (which calculates function γ), TestD (which calculates function δ), TestE (which calculates function ζ), TestF and TestG.

TestA calculates function α using TestB which calculates function β incorporating the results of the Theorem 1. TestB calculates function β using TestC which calculates function γ incorporating the results of the Theorem 2 and so on (for the details see the pseudocode available on the internet (http://www.pmfst.hr/~vukicevi/ProjEngIndex.htm)

At the end (in the time that is proportional or less then the product of

$$\min\{m_{12}, m_{13}, m_{23}\} \cdot \{m_{13}/2, m_{23}\})$$

we get a required solution (it can be seen that there are just two loops: line 2.1 in TestA and line 3 in the TestC which directly implies the complexity of the result).

4. Conclusion

The problem of determining weather there is a graph with the prescribed thorns and bond connectivities is not simple. Namely, there is extremely large family of graphs that should be taken under consideration. Note that the number of graphs is non-polynomial in the number of its vertices. Each solution based on the non-polynomial algorithm is intractable for graphs with large number of vertices (basically non-polynomial algorithms are suitable for graphs of (say) up to 15 vertices). Here, we give the theorems that enable different approach to this problem. Namely, instead of examining all graphs, we have necessary and sufficient conditions on numbers $i_1, i_2, i_3, i_4, i_5, i_6, i_7, i_8, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}$ for the existence of the corresponding graph. In this way, we obtained an algorithm which number of operations is proportional to $\min\{m_{12}, m_{13}, m_{23}\} \cdot \{m_{13}/2, m_{23}\}$. Hence, the non-efficient polynomial algorithm is replaced by the very efficient polynomial algorithm. This algorithm works instantly even for graphs with few hundred vertices and is capable to work with graphs of even much larger size.

References

[1] L. Bytautas, D. Bonchev and D.J. Klein, MATCH Commun. Math. Comput. Chem. 44 (2001) 31-40.

[2] D. Bonchev and D.J. Klein, Croat. Chem. Acta 75 (2002) 613-620.

[3] A. Cayley, Phil. Mag. 47 (1874) 444-446.

[4] I. Gutman, D. Vidović and L. Popović, J. Chem. Soc., Faraday Trans. 94 (1998) 857-860.

[5] I. Gutman, A.A. Toroporov and A.P. Toropova, MATCH Commun. Math. Comput. Chem. 53 (2005) 215-224.

[6] I. Gutman, B. Furtula, A.A. Toroporov and A.P. Toropova, MATCH Commun. Math. Comput. Chem. 53 (2005) 225-230.

[7] D. Vukičević, A. Miličević, S. Nikolić, J. Sedlar and N. Trinajstić, Arkivoc 2005 (X) 45-49.
http://www.arkat-usa.org/

[8] T.B.C. McLeish, Math. Chem. 6 (1999) 265-315.

[9] T.C.B. McLeish, In Topology in Chemistry, Mathematical Chemistry Series, Vol. 6, Edited by D. Bonchev and D.H. Rouvray (Gordon & Breach, Reading, 1999) 265-315.

[10] A.H. Widman and G.R. Davies, Comput. Theoret. Polym. Sci. 8 (1998) 191-199.

[11] M.V. Diudea and G. Katona, Adv. Dendritic Macromol. 4 (1999) 135-201.

[12] F. Harary, *Graph Theory*, 2nd printing (Addison-Wesley, Reading, MA, 1971).

[13] R.J. Wilson, *Introduction to Graph Theory* (Oliver and Boyd, Edinburgh, 1972).

[14] D. Veljan, *Combinatorics and Discrete Mathematics* (Algorithm, Zagreb, 2001)