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Compact Valence Sequences for Molecules with Single, Double and Triple Covalent Bonds. II. Graphs with Non-trivial Cycles*

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Molecular graphs able to model covalent multiple bonds are called plerographs. For such graphs, with single, double and triple edges, compact degree sequences (n_1, n_2, n_3, n_4), where n_i, i = 1, 2, 3, 4 denote the number of vertices of degree i, are defined. Investigations are extended to necessary and sufficient conditions on (n_1, n_2, n_3, n_4) for the existence of graph G such that G has n_1, n_2, n_3 and n_4 vertices of degrees 1, 2, 3 and 4. Namely, graphs with nontrivial cycles with at least three vertices are allowed.

INTRODUCTION

Molecules are conveniently represented by two types of molecular graphs:[1–4] plerographs (in which each atom is represented by a vertex) and kenographs (in which hydrogen atoms are suppressed). Like in the prequel[5] to this paper, here we consider plerographs as well. Plerographs were presented in the original paper of Cayley.[1] For recent studies of plerographs see Refs. 2 and 3.

The valence of the molecule is the number of bonds emanating from the observed atom. Most molecules have valencies of at most 4 and hence we restrict (as in our previous paper)[5] our attention to plerographs of such molecules. In the prequel,[5] we allowed only molecules without loops and without nontrivial cycles (*i.e.*, molecules that may have only »cycles« of length 2 or molecules that would be transformed to trees by replacement of all multiple edges by single edges). Here, we supersede this restriction and observe all connected graphs without loops. This includes a much wider class of molecules (in particular, all molecules containing benzenoid rings). Similarly as in the prequel,[5] we denote by Γ_1^o, Γ_{12}^o, Γ_{13}^o and Γ_{123}^o, respectively, the set of plerographs containing single bonds, containing single and/or double bonds, containing single and/or triple bonds and containing single and/or double bonds and/or triple bonds. Here, we only put o as a superscript to emphasize that we allow nontrivial cycles of length at least three.

The bonding topology of molecules can be characterized in a variety of ways. In papers[6–9] sequences of

* Dedicated to Professor Haruo Hosoya in happy celebration of his 70th birthday.

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valence connectivities were analyzed. Here, we analyze degree sequences. The degree of vertex i of graph G, $d_i = d_i$ (G), equals the number of edges incident to i, while for plerographs it fully coincides with the valence of the i-th atom of a molecule represented by G. Let v(G) denote the number of vertices of G and e(G) stand for the number of bonds (taking into account their multiple character) in G. The monotonic nondecreasing sequence of vertex degrees is called a degree sequence, *i.e.,* for graphs treated here it is a sequence of length v(G) with entries 1, 2, 3 and 4. The degree sequence can be contracted into a compact degree sequence, υ(G) (the compact valence sequence) of the form $\upsilon = \upsilon(G) = (n_1, n_2, n_3, n_4)$, where n_j, j = 1, 2, 3, 4, denotes how frequently vertex degree equal to j occurs in a degree sequence. Obviously, a compact degree sequence represents the partition of vertices in G in (here four) classes of vertices having the same degree.

To each graph G, we can ascribe the 4-tuple υ(G), but the opposite generally does not hold, *e.g.,* no graph exists for 4-tuple (3,0,0,0).

In the present paper, we address three problems analogous to the problems addressed in the prequel:[5]

i) for a given 4-tuple (n_1, n_2, n_3, n_4) find necessary and sufficient conditions for $\Gamma_{12}^o(n_1, n_2, n_3, n_4) \neq \varnothing$.
ii) solve the same as above for $\Gamma_{13}^o(n_1, n_2, n_3, n_4)$,
iii) solve the same for $\Gamma_{123}^o(n_1, n_2, n_3, n_4)$.

Like in the prequel,[5] these problems are solved here and formulated in three theorems.

Preliminary to further considerations, let e_2(G), e_3(G), Δ(G) and Δ'(G) denote the number of double bonds, triple bonds, maximal vertex degree of G and second maximal vertex degree of G, respectively. Single edge, double edge and triple edge are defined as in the prequel.

MAIN RESULTS

We start with several auxiliary Lemmas:

Lemma 1. – Let $\Gamma_{12}^o(n_1, n_2, n_3, n_4) \neq \varnothing$ such that $n_1 \leq n_3 + 2n_4$, then $\Gamma_{12}^o(n_1 + 2, n_2, n_3, n_4) \neq \varnothing$.

Proof: Let $G \in \Gamma_{12}^o(n_1, n_2, n_3, n_4)$. Simple calculation shows that graph G either contains a cycle or double edge, because otherwise $n_1 + 2n_2 + 3n_3 + 4n_4 \leq 2(n_1 + n_2 + n_3 + n_4 - 1)$. Let e be an edge of the cycle or one of two edges in a double edge. Let u and v be endvertices of e. Let G' be a graph obtained by deletion of edge e and adding two pendant vertices to u and v. Then, $G' \in \Gamma_{12}^o(n_1 + 2, n_2, n_3, n_4)$. ■

Iterative application of this lemma implies:

Lemma 2. – Let $\Gamma_{12}^o(n_1, n_2, n_3, n_4) \neq \varnothing$ such that $n_1 + 2k \leq n_3 + 2n_4 + 2$ where $k \in N_0$, then $\Gamma_{12}^o(n_1 + 2k, n_2, n_3, n_4) \neq \varnothing$. ■

We omit the proofs of the following 3 Lemmas, because they are completely analogous to the proofs of Lemmas in Ref. 5.

Lemma 3. – Let $G \in \Gamma_{12}^o(n_1, n_2, n_3, n_4)$ be a graph that contains at least one edge and let $k \in N$. Then, there is a graph $G' \in \Gamma_{12}^o(n_1, n_2 + k, n_3, n_4)$ that contains at least one single edge. ■

Lemma 4. – Let $G \in \Gamma_{12}^o(n_1, n_2, n_3, n_4)$ be a graph that contains at least one edge and let $k \in N$. Then, there is a graph $G' \in \Gamma_{12}^o(n_1, n_2, n_3 + 2k, n_4)$ that contains at least one single edge. ■

Lemma 5. – Let $G \in \Gamma_{12}^o(n_1, n_2, n_3, n_4)$ be a graph that contains at least one double edge and let $k \in N$. Then, there is a graph $G' \in \Gamma_{12}^o(n_1, n_2, n_3, n_4 + k)$ that contains at least one double edge. ■

Let us prove:

Theorem 6. – Let $n_1, n_2, n_3, n_4 \in N_0$. Then, $\Gamma_{12}^o(n_1, n_2, n_3, n_4) \neq \varnothing$ if and only if the following holds:

1) $n_1 \equiv n_3 \pmod 2$;
2) $n_1 \leq n_3 + 2n_4 + 2$;
3) $2\Delta \leq n_1 + 2n_2 + 3n_3 + 4n_4$;
4) $2\Delta + 2\Delta' \leq n_1 + 2n_2 + 3n_3 + 4n_4 + 4$.

Proof: Suppose that $G \in \Gamma_{12}^o(n_1, n_2, n_3, n_4)$. From handshaking Lemma it follows 1). Since $e(G) \geq v(G) - 1$, it follows that $\frac{n_1 + 2n_2 + 3n_3 + 4n_4}{2} \geq n_1 + n_2 + n_3 + n_4 - 1$, which implies 2). We have $2\Delta \leq 2 \cdot e(G) = n_1 + 2n_2 + 3n_3 + 4n_4$ and $2\Delta + 2\Delta' - 4 \leq 2 \cdot e(G) \leq n_1 + 2n_2 + 3n_3 + 4n_4$; hence 3) and 4) hold.

Now, let us prove the opposite implication. Distinguish two cases:

CASE 1: $n_2 + n_3 + n_4 \geq 3$.

Denote by $G_1, G_2, \ldots, G_{12}$ respectively, the graphs in the following figure:

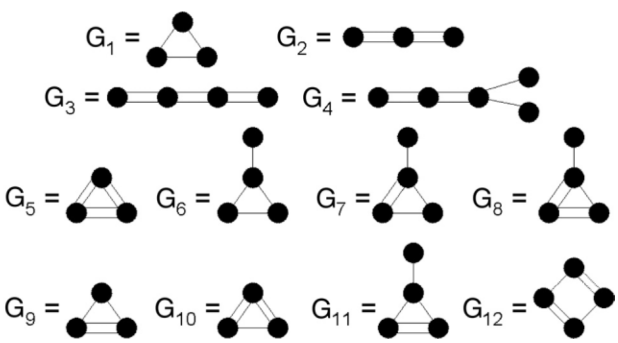

Figure 1. Graphs $G_1, G_2, \ldots, G_{12}$.

Distinguish 9 subcases:

SUBCASE 1.1: $n_3 = 0$ and $n_4 = 0$.

Note that $n_2 \geq 3$. The claim follows from graph G_1 and Lemmas 2 and 3. Namely, from Lemma 2, it follows that there is a graph G_1' such that $\upsilon(G) = (0, n_2, 0, 0)$ and then from Lemma 3, it follows that there is a graph G_1'' such that $\upsilon(G) = (n_1, n_2, 0, 0) \equiv (n_1, n_2, n_3, n_4)$.

SUBCASE 1.2: $n_3 = 0$, $n_4 = 1$.

Note that $n_2 \geq 2$. The claim follows from graph G_2 and Lemmas 2 and 3.

SUBCASE 1.3: $n_3 = 0$, $n_4 = 2$.

Note that $n_2 \geq 1$ and that relation 3) implies that either $n_2 \geq 2$ or $n_1 \geq 2$. In the first case, the claim follows from graph G_3 and Lemmas 2 and 3 and in the second case the claim follows from graph G_4 and Lemmas 2 and 3.

SUBCASE 1.4: $n_3 = 0$, $n_4 \geq 3$.

The claim follows from graph G_5 and Lemmas 2, 3 and 5.

SUBCASE 1.5: $n_3 = 1$, $n_4 = 0$.

Note that $n_2 \geq 2$ and $n_1 \geq 1$. The claim follows from graph G_6 and Lemmas 2 and 3.

SUBCASE 1.6: $n_3 = 1$, $n_4 = 1$.

Note that n_1, $n_2 \geq 1$. The claim follows from graph G_7 and Lemmas 2 and 3.

SUBCASE 1.7: $n_3 = 1$, $n_4 \geq 2$.

Note that $n_1 \geq 1$. The claim follows from graph G_8 and Lemmas 2, 3 and 5.

SUBCASE 1.8: $n_3 = 2$.

Note that either $n_2 \geq 1$ or $n_4 \geq 1$. In the first case, the claim follows from graph G_9 and Lemmas 2, 3 and 5; and in the second case the claim follows from graph G_{10} and Lemmas 2, 3 and 5.

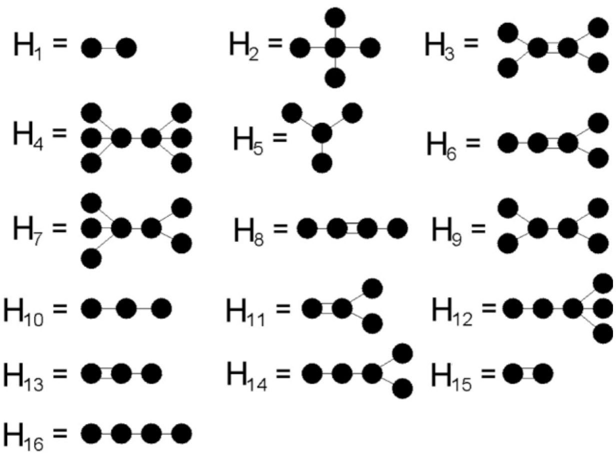

Figure 2. Graphs H_1,..., H_{16}.

SUBCASE 1.9: $n_3 \geq 3$.

If n_3 is odd, then n_1 is odd, too; and the claim follows from graph G_{11} and Lemmas 2, 3, 4, and 5. If n_3 is even, then the claim follows from graph G_{12} and Lemmas 2, 3, 4, and 5.

CASE 2: $n_2 + n_3 + n_4 \leq 2$.

Denote by H_1,..., H_{16} respectively, the graphs in the Figure 2.

Analyses of all the possible cases are presented by the following table (the fourth column gives the possible values of n_1 implied by relations 1) – 4); the fifth column contains graphs that realize the observed cases):

n_2	n_3	n_4	n_1	graph(s)
0	0	0	2	H_1
0	0	1	4	H_2
0	0	2	4,6	H_3, H_4
0	1	0	3	H_5
0	1	1	3,5	H_6, H_7
0	2	0	2,4	H_8, H_9
1	0	0	2	H_{10}
1	0	1	2,4	H_{11}, H_{12}
1	1	0	1,3	H_{13}, H_{14}
2	0	0	0,2	H_{15}, H_{16}

All the cases are exhausted and the theorem is proved. ■

Theorem 7. – Let $n_1, n_2, n_3, n_4 \in N_0$. Then, $\Gamma^{o}_{123}(n_1, n_2, n_3, n_4) \neq \varnothing$ if and only if the following holds:

1) $n_1 \equiv n_3 \pmod 2$;
2) $n_1 \leq n_3 + 2n_4 + 2$;
3) $2\Delta \leq n_1 + 2n_2 + 3n_3 + 4n_4$;
4) $2\Delta + 2\Delta' \leq n_1 + 2n_2 + 3n_3 + 4n_4 + 6$.

Proof: Suppose that $G \in \Gamma^{o}_{123}(n_1, n_2, n_3, n_4)$. Relations 1) – 3) can be proved in the same way as in the proof of Theorem 6 and from $2\Delta + 2\Delta' - 6 \leq 2 \cdot e(G) \leq n_1 + 2n_2 + 3n_3 + 4n_4$ follows 4).

Now, let us prove the opposite inequality. If $2\Delta + 2\Delta' \leq n_1 + 2n_2 + 3n_3 + 4n_4 + 4$, then $\varnothing \neq \Gamma^{o}_{12}(n_1, n_2, n_3, n_4) \subseteq \Gamma^{o}_{123}(n_1, n_2, n_3, n_4)$. Hence, it is sufficient to prove the claim when $2\Delta + 2\Delta' = n_1 + 2n_2 + 3n_3 + 4n_4 + 6$. Note that in this case the quadruple (n_1, n_2, n_3, n_4) is one of the following (0,0,2,0), (1,0,1,1), (2,0,0,2) or (0,1,0,2). In each case, the respective graphs can be easily constructed. ■

Theorem 11 from Ref. 9 can be reformulated as:

Theorem 8. – Let $n \geq 3$ and let n_1, n_2, n_3 and n_4 be non-negative natural numbers such that $n_1 + n_2 + n_3 + n_4 = n$. Then $\Gamma_1(n_1, n_2, n_3, n_4) \neq \varnothing$ if and only if the following conditions hold:

1) $n_3 + 2n_4 \geq n_1 - 2$;
2) $\frac{3n_3+4n_4-n_1}{2} - n_2 \leq \binom{n_3+n_4}{2}$;
3) $n_1 + n_3$ is an even number;
4) If $n_3 + n_4 = 1$, then $n_2 \geq 3n_3 + 4n_4 - n_1$. ■

Let us prove:

Lemma 9. – Let $n_1, n_2, n_3, n_4 \in N_0$ such that $n_1 + n_2 + n_3 + n_4 \geq 3$. There is a graph $G' \in \Gamma_{13}^{o}(n_1, n_2, n_3, n_4)$ if and only if there are $x, y \in N_0$, such that $G \in \Gamma_1^{o}(n_1 + x, n_2, n_3 - sx, n_4 - x - 2y)$.

Proof: Suppose that $G' \in \Gamma_{13}^{o}(n_1, n_2, n_3, n_4)$. Note that each triple bond connects either vertices of degrees 3 and 4 (denote the number of such bonds by x) or two vertices of degree 4 (denote number of such bonds by y). Let G be the graph obtained from graph G' by elimination of all triple bonds by the following two replacements:

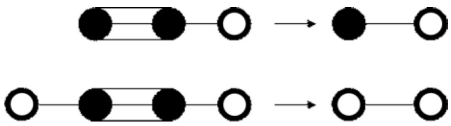

Figure 3. Replacements in Graph G.

Graph G is an element of $\Gamma_1^{o}(n_1 + x, n_2, n_3 - x, n_4 - x - 2y)$.

Now, let us prove the opposite implication. Suppose that $G \in \Gamma_1^{o}(n_1 + x, n_2, n_3 - x, n_4 - x - 2y)$ for some x and y. Add to x vertices (in G) of degree 1 a single neighbor connected by a triple edge and replace one single edge by the detail depicted below:

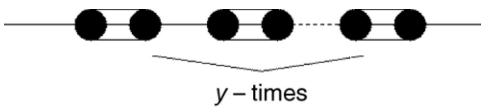

Figure 4. The detail that replaces the edge.

In this way, graph $G' \in \Gamma_{13}^{o}(n_1, n_2, n_3, n_4)$ is constructed. ■

Combining Theorem 8 and Lemma 9, one obtains:

Lemma 10. – Let $n_1, n_2, n_3, n_4 \in N_0$ be such that $n_1 + n_2 + n_3 + n_4 \geq 3$. There is a graph $G \in \Gamma_{13}^{o}(n_1, n_2, n_3, n_4)$ if and only if there are $x, y \in N_0$ such that:

1) $n_3 + 2n_4 - 4x - 4y \geq n_1 - 2$;
2) $\frac{3n_3+4n_4-n_1-8x-8y}{2} - n_2 \leq \binom{n_3+n_4-2x-2y}{2}$;
3) $n_1 + n_3$ is an even number;
4) If $n_3 + n_4 - 2x - 2y = 1$, then $n_2 \geq 3n_3 + 4n_4 - n_1 - 8x - 8y$;
5) $x \leq n_3$;
6) $x + 2y \leq n_4$. ■

We need another auxiliary result:

Lemma 11. – Let $w, n_3, n_4 \in N_0$. There are numbers $x, y \in N_0$ such that $x + y = w$, $x \leq n_3$, and $x + 2y \leq n_4$ if and only if $w \leq (n_3 + n_4) / 2$ and $w \leq n_4$.

Proof: Suppose that $x \leq n_3$ and $x + 2y \leq n_4$. Note that $w = x + y \leq x + 2y \leq n_4$ and that $w = (x + (x + 2y))/2 \leq (n_3 + n_4)/2$.

Let us prove the opposite implication. Distinguish two cases:

CASE 1: $w \leq n_3$.
Just take $x = w$ and $y = 0$.
CASE 2: $w \geq n_3$.
Just take $x = n_3$ and $y = w - n_3$. ■

Combining Lemmas 10 and 11, we get:

Lemma 12. – Let $n_1, n_2, n_3, n_4 \in N_0$ be such that $n_1 + n_2 + n_3 + n_4 \geq 3$. There is a graph $G \in \Gamma_{13}^{o}(n_1, n_2, n_3, n_4)$ if and only if there is $w \in N_0$ such that:

1) $n_3 + 2n_4 - 4w \geq n_1 - 2$;
2) $\frac{3n_3+4n_4-n_1-8w}{2} - n_2 \leq \binom{n_3+n_4-2w}{2}$;
3) $n_1 + n_3$ is an even number;
4) If $n_3 + n_4 - w = 1$, then $n_2 \geq 3n_3 + 4n_4 - n_1 - 8w$;
5) $w \leq (n_3 + n_4) / 2$;
6) $w \leq n_4$. ■

Last Lemma can be reformulated as:

Lemma 13. – Let $n_1, n_2, n_3, n_4 \in N_0$ be such that $n_1 + n_2 + n_3 + n_4 \geq 3$. Then, $\Gamma_{13}^{o}(n_1, n_2, n_3, n_4) \neq \varnothing$ if and only if there is $w \in N_0$ such that:

1) $w \leq (n_3 + 2n_4 - n_1 + 2) / 4$;
2) $25 - 4 \cdot n_1 - 8 \cdot n_2 - 4 \cdot n_3 < 0$ or
$w \leq (-5 - \sqrt{25-4\cdot n_1-8\cdot n_2-4\cdot n_3}+2n_3+2n_4)/4$ or
$w \geq (-5 + \sqrt{25-4\cdot n_1-8\cdot n_2-4\cdot n_3}+2n_3+2n_4)/4$;
3) $n_1 + n_3$ is an even number;
4) $n_3 + n_4 - w \neq 1$ or $w \geq (3n_3 + 4n_4 - n_1 - n_2) / 8$;
5) $w \leq (n_3 + n_4) / 2$;
6) $w \leq n_4$;
7) $w \geq 0$. ■

Denote by $[a, b]_z$ the set of integers x such that $a \leq x \leq b$. From Lemma 13, it easily follows that:

Theorem 14. – Let n_1, n_2, n_3, $n_4 \in N_0$ be such that $n_1 + n_2 + n_3 + n_4 \geq 3$. Then, $\Gamma^{o}_{13}(n_1, n_2, n_3, n_4) \neq \varnothing$ if and only if $n_1 + n_3$ is an even number and one of the following holds:

1) $$\max\left\{0, \left\lceil (3n_3 + 4n_4 - n_1 - n_2)/8 \right\rceil\right\} \leq \min\left\{\begin{matrix} \left\lfloor (n_3 + 2n_4 - n_1 + 2)/4 \right\rfloor, \left\lfloor (n_3 + n_4)/2 \right\rfloor, n_4 \\ \left\lfloor (-5 + 2n_3 + 2n_4 - \sqrt{25 - 4\cdot n_1 - 8\cdot n_2 - 4\cdot n_3})/4, \right\rfloor, \end{matrix}\right\};$$

2) $$\left[0, \min\left\{\begin{matrix} \left\lfloor (n_3 + 2n_4 - n_1 + 2)/4 \right\rfloor, \left\lfloor (n_3 + n_4)/2 \right\rfloor, n_4, \\ \left\lfloor (-5 + 2n_3 + 2n_4 - \sqrt{25 - 4\cdot n_1 - 8\cdot n_2 - 4\cdot n_3})/4, \right\rfloor \end{matrix}\right\}\right]_Z \setminus \{1 - n_3 - n_4\} \neq \varnothing;$$

3) $$\max\left\{\begin{matrix} 0, \left\lceil (3n_3 + 4n_4 - n_1 - n_2)/8 \right\rceil, \\ \left\lceil (-5 + 2n_3 + 2n_4 + \sqrt{25 - 4\cdot n_1 - 8\cdot n_2 - 4\cdot n_3})/4 \right\rceil \end{matrix}\right\} \leq \min\left\{\begin{matrix} \left\lfloor (n_3 + 2n_4 - n_1 + 2)/4 \right\rfloor, \\ \left\lfloor (n_3 + n_4)/2 \right\rfloor, n_4 \end{matrix}\right\};$$

4) $$\left[\begin{matrix} \max\left\{0, \left\lceil (-5 + 2n_3 + 2n_4 + \sqrt{25 - 4\cdot n_1 - 8\cdot n_2 - 4\cdot n_3})/4 \right\rceil\right\} \\ \min\left\{\begin{matrix} \left\lfloor (n_3 + 2n_4 - n_1 + 2)/4 \right\rfloor, \\ \left\lfloor (n_3 + n_4)/2 \right\rfloor, n_4 \end{matrix}\right\} \end{matrix}\right]_Z \setminus \{1 - n_3 - n_4\} \neq \varnothing;$$

5) $25 - 4 \cdot n_1 - 8 \cdot n_2 - 4 \cdot n_3 < 0$ and

$$\left[\max\left\{0, \left\lceil (3n_3 + 4n_4 - n_1 - n_2)/8 \right\rceil\right\} \leq \min\left\{\left\lfloor (n_3 + 2n_4 - n_1 + 2)/4 \right\rfloor, \left\lfloor (n_3 + n_4)/2 \right\rfloor, n_4\right\}\right];$$

6) $$25 - 4 \cdot n_1 - 8 \cdot n_2 - 4 \cdot n_3 < 0 \text{ and } \left[0, \min\left\{\begin{matrix} \left\lfloor (n_3 + 2n_4 - n_1 + 2)/4 \right\rfloor, \\ \left\lfloor (n_3 + n_4)/2 \right\rfloor, n_4 \end{matrix}\right\}\right]_Z \setminus \{1 - n_3 - n_4\} \neq \varnothing. \blacksquare$$

CONCLUSIONS

Degree sequences are contracted here to 4-tuples (n_1, n_2, n_3, n_4) where n_i, i = 1, 2, 3, 4, stands for the number of vertices of degree i. In defining 4-tuples we allow that vertices could be connected by single, double and triple edges. In such a way, in contrast to most of the mathematical chemistry literature, we are able to model multiple covalent bonds of most molecules of chemical interest. Here, we determine the necessary and sufficient conditions on 4-tuple (n_1, n_2, n_3, n_4) for the existence of a graph G that may contain cycles of length at least three such that G has n_1, n_2, n_3 and n_4 vertices of degree 1, 2, 3 and 4. Hence, a much larger class of graphs is observed here than in the prequel to this paper. Hence, both of these papers further the results given in Kier *et al.*,[10] Skvortsova *et al.*,[11] J. K. Senior,[12,13] and Bytautas and Klein.[14–16]

As degree sequences (or equivalently 4-tuples) have already served to define a number of molecular descriptors[17] able to correlate molecular properties,[18] the results achieved here could be of interest when one is interested in taking into account multiple covalent bonds in molecules.

As a very simple example, we illustrate this by the sequence (6,0,0,6) that represents the molecule with 6 vertices of degree 4 and 6 vertices of degree 1. This molecule corresponds to benzene (note that one has to take into account double bonds in Kekulé structures and a non-trival cycle of length 6).

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SAŽETAK

Kompaktni valentni nizovi molekula s jednostrukim, dvostrukim i trostrukim kovalentnim vezama. II. Grafovi s netrivijalnim ciklusima

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Molekularni grafovi koji mogu modelirati višestruke kovalentne veze zovu se plerografovi. Za takve grafove s jednostrukim, dvostrukim i trostrukim vezama definiran je kompaktni niz stupnjeva (n_1, n_2, n_3, n_4), gdje n_i, i = 1, 2, 3, 4 predstavlja broj vrhova stupnja i. Ovime je nastavljeno istraživanje nužnih i dovoljnih uvjeta na (n_1, n_2, n_3, n_4) za postojanje grafa G, takvog da G ima n_1, n_2, n_3 i n_4 vrhova stupnja 1, 2, 3, 4. Naime, ovdje su dopušteni i grafovi s netrivijalnim ciklusima (ciklusima s barem 3 vrha).