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Compact Valence Sequences for Molecules with Single, Double and Triple Covalent Bonds*

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Molecular graphs able to model covalent multiple bonds are called plerographs. For such graphs with single, double and triple edges, we define here the compact degree sequence (n_1, n_2, n_3, n_4), where n_i, i = 1, 2, 3, 4 denote the number of vertices of degree i. We have found the necessary and sufficient conditions (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, and have formulated the findings into three theorems.

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). Here, we consider plerographs which, apart from the original paper of Cayley,[1] have been only recently reviewed in chemical literature.[2–4] In plerographs according to Cayley and adopted here, the number of bonds emanating from an atom equals its valence. For most molecules, it is sufficient to consider valencies of up to 4. In this paper, we pay attention to plerographs of such molecules, *i.e.*, we treat the connected graphs without loops having single, double, and triple covalent bonds. By Γ_1, Γ_{12}, Γ_{13} and Γ_{123} we denote 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, respectively.

The bonding topology of molecules can be characterized in a variety of ways.[5] One of them is offered by degree sequences. The degree of vertex i of graph G, $d_i = d_i$ (G) equals the number of edges incident to i, and for plerographs fully coincides with the valence of the i-th atom of a molecule represented by G. Let υ(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 non-decreasing sequence of vertex degrees is called a degree sequence, *i.e.*, for graphs treated here it is a sequence of length υ(G) with entries 1, 2, 3 and 4. The degree sequence can be contracted into a compact degree sequence, υ(G) (compact valence

* Dedicated to Dr. Edward C. Kirby in happy celebration of his 70th birthday.

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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 the vertex degree equal to j occurs in a degree sequence. Obviously, the compact degree sequence represents a partition of vertices in G in (here four) classes of vertices having the same degree.

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

In the present paper, we address the following three problems:

1) for a given 4-tuple (n_1, n_2, n_3, n_4) find the necessary and sufficient conditions for the existence of graph $G \in \Gamma_{12}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$;
2) solve the same as above for $G \in \Gamma_{13}$;
3) solve the same for $G \in \Gamma_{123}$.

These problems are solved here and formulated in three theorems.

Preliminary to further considerations, let denote by $e_2(G)$, $e_3(G)$ and $\Delta(G)$ the number of double bonds, triple bonds and the maximal vertex degree of G, respectively.

MAIN RESULTS

Bonds and edges are in one to one correspondence: if there is just one edge e that connects vertices x and y, then we say that e is a single edge, if there are two edges e' and e'' that connect vertices x and y, then we say that the pair e' and e'' is a double edge, and if there are three edges e', e'' and e''' that connect vertices x and y, then we say that a triplet e', e'' and e''' is a triple edge.

Let us give a few auxiliary results:

Lemma 1. – Let $G \in \Gamma_{12}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$. Then, $e_2(G) = (n_3 + 2n_4 - n_1 + 2)/2$.

Proof. The claim follows directly from this equation (implied by hand-shaking Lemma):

$$4e_2(G) + 2(n_1 + n_2 + n_3 + n_4 - 1 - e_2(G)) = n_1 + 2n_2 + 3n_3 + 4n_4. \blacksquare$$

Note that number 4 stands, because each double edge contributes 4 to the sum of vertex degrees (it contributes 2 to the degree of its two adjacent vertices).

Lemma 2. – Let $G \in \Gamma_{12}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$, and let $k \in N_0$ (where N_0 denotes the set of natural number together with 0) such that $k \le e_2(G)$. Then, there is a graph $G' \in \Gamma_{12}$ such that $\upsilon(G') = (n_1 + 2k, n_2, n_3, n_4)$.

Proof. Select arbitrary k double edges. Graph G' is obtained by replacing each of them by a single edge and adding to each of its endvertices one neighbor of degree 1. ■

Lemma 3. – Let $G \in \Gamma_{12}$ be a graph that contains at least one single edge such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$. Then, there exists a graph $G' \in \Gamma_{12}$ that contains at least one single edge such that $\upsilon(G') = (n_1, n_2 + 1, n_3, n_4)$.

Proof. Graph G' is obtained from graph G by replacing arbitrary edge with an item depicted below:

Figure 1. Item that replaces an edge of G.

■

This implies:

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

Let us prove:

Lemma 5. – Let $G \in \Gamma_{12}$ be a graph that contains at least one single edge such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$. Then, there is a graph $G' \in \Gamma_{12}$ that contains at least one single edge such that $\upsilon(G') = (n_1, n_2, n_3 + 2, n_4)$.

Proof. Graph G' is obtained from graph G by replacing a single edge with an item shown below:

Figure 2. Item that replaces an edge of G.

■

From this Lemma, it easily follows that:

Lemma 6. – Let $G \in \Gamma_{12}$ be a graph that contains at least one single edge such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ and let $k \in N$. Then there is a graph $G' \in \Gamma_{12}$ that contains at least one single edge such that $\upsilon(G') = (n_1, n_2, n_3 + 2k, n_4)$.

Now, we prove:

Lemma 7. – Let $G \in \Gamma_{12}$ be a graph that contains at least one double edge such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$. Then, there is a graph $G' \in \Gamma_{12}$ that contains at least one double edge such that $\upsilon(G') = (n_1, n_2, n_3, n_4 + 1)$.

Proof. Graph G' is obtained from graph G by replacing a double edge with an item given below:

Figure 3. Item that replaces a double edge of G.

■

It follows that:

Lemma 8. – Let $G \in \Gamma_{12}$ be a graph that contains at least one double edge such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ and let

$k \in N$. Then, there is a graph G' $\in \Gamma_{12}$ that contains at least one double edge such that $\upsilon(G') = (n_1, n_2, n_3, n_4 + k)$.

Now, we can prove our first theorem:

Theorem 9. – Let $n_1, n_2, n_3, n_4 \in N_0$. Then, there is a graph G $\in \Gamma_{12}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ if and only if $n_2 = n_3 = n_4 = 0$ and $n_1 = 2$; or the following holds:

1) $n_1 = n_3 \pmod 2$
2) $n_1 \leq n_3 + 2n_4 + 2$
3) if $n_3 = 0$, then $n_1 + 2n_2 \geq 4$
4) if $n_3 \geq 1$, then $n_1 + n_2 \geq 2$
5) $n_1 = n_3 = 0 \Rightarrow n_2 = 2$.

Proof. First, let us prove necessity. If $n_2 = n_3 = n_4 = 0$ and $n_1 = 2$, the claim is trivial, so suppose that 1) – 5) hold. Let us distinguish six cases:

CASE 1: $n_3 = 0$, $n_1 = 0$.

Note that then $n_2 = 2$. The claim follows from graph P$_2$':

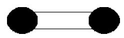

Figure 4. Graph P$_2$'.

and Lemma 8.

CASE 2: $n_3 = 0$, $n_1 = 2$.

Note that $n_2 \geq 1$. If $n_4 = 0$, the claim is proved by considering graph H$_5$:

Figure 5. Graph H$_5$.

and Lemma 4. If $n_4 \geq 1$, the claim follows looking at graph H$_6$:

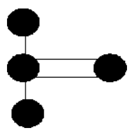

Figure 6. Graph H$_6$.

and Lemmas 4 and 8.

CASE 3: $n_3 = 0$, $n_1 \geq 4$.

Note that $n_4 \geq 1$. If $n_4 = 1$, then $n_1 = 4$. From graph H$_7$:

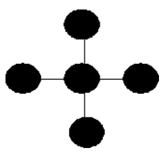

Figure 7. Graph H$_7$.

and Lemma 4, the claim follows. Suppose that $n_4 \geq 2$. From graph H$_8$:

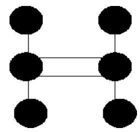

Figure 8. Graph H$_8$.

and Lemmas 4 and 8, it follows that there is a graph G' such that $\upsilon(G') = (4, n_2, n_3, n_4)$. Note that $4 \leq n_1 \leq n_3 + 2n_4 + 2$ and n_1 is an even number. Also, note that $e_2(G') = (n_3 + 2n_4 - 2) / 2$ and that $(n_1 - 4) / 2 \leq (n_3 + 2n_4 - 2) / 2$. Therefore, from Lemma 2 it follows that there is a graph G such that $\upsilon(G) = (4 + 2\,(n_1 - 4) / 2, n_2, n_3, n_4) = (n_1, n_2, n_3, n_4)$.

CASE 4: $n_3 \geq 1$, $n_1 = 1$.

Note that $n_2 \geq 1$ and that n_3 is odd. From graph H$_9$:

Figure 9. Graph H$_9$.

and Lemmas 4, 6 and 8, the claim follows.

CASE 5: $n_3 \geq 1$, $n_1 \geq 2$, n_1 and n_3 are even.

From graph H$_{10}$:

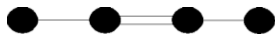

Figure 10. Graph H$_{10}$.

and Lemmas 4, 6 and 8, it follows that there is a graph G' such that $\upsilon(G') = (2, n_2, n_3, n_4)$. Note that $2 \leq n_1 \leq n_3 + 2n_4 + 2$ and n_1 is an even number. Also, note that $e_2(G') = (n_3 + 2n_4 - 2) / 2$ and that $(n_1 - 2) / 2 \leq (n_3 + 2n_4) / 2$. Wherefrom, by Lemma 2, it follows that there is a graph G such that $\upsilon(G) = (2 + 2\,(n_1 - 2) / 2, n_2, n_3, n_4) = (n_1, n_2, n_3, n_4)$.

CASE 6: $n_3 \geq 1$, $n_1 \geq 2$, n_1 and n_3 are odd.

Suppose that $n_4 = 0$. From graph H$_{11}$:

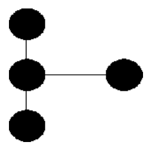

Figure 11. Graph H$_{11}$.

and Lemmas 4 and 6, it follows that there is graph G' such that $\upsilon(G') = (3, n_2, n_3, n_4)$. Graph G such that $\upsilon(G) =$

(n_1, n_2, n_3, n_4) can be constructed analogously to the above. Now, suppose that $n_4 \geq 1$. Graph H_{12}:

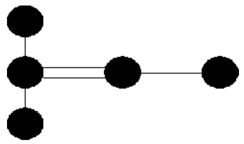

Figure 12. Graph H_{12}.

and Lemmas 4, 6 and 8 imply that there is graph G' such that υ(G') = (3, n_2, n_3, n_4). Graph G such that υ(G) = (n_1, n_2, n_3, n_4) can be constructed analogously as before.

All the cases are now exhausted and necessity is proved. Now, let us prove sufficiency. If G is a path of length 1, the claim is trivial, so suppose that G is not a path of length 1. From the Handshaking Lemma (the number of vertices with an odd degree is even) follows that $n_1 = n_3$ (mod 2). From the fact that every molecular graph is connected, it follows that $e(G) \geq n(G) - 1$, which is equivalent to

$$n_1 + 2n_2 + 3n_3 + 4n_4 \geq 2\ (n_1 + n_2 + n_3 + n_4 - 1);$$
$$n_1 \leq n_3 + 2n_4 + 2.$$

Suppose that $n_3 = 0$. We have:

$$n_1 + 2n_2 + 4n_4 = 2(n_1 + n_2 + n_4 - 1 - e_2(G)) + 4e_2(G).$$

Note that $e_2(G) \leq n_2 + n_4 - 1$, hence

$$n_1 + 2n_2 + 4n_4 \leq$$
$$2(n_1 + n_2 + n_4 - 1 - (n_2 + n_4 - 1)) + 4(n_2 + n_4 - 1).$$

From here, 3) easily follows.

Now, suppose that $n_3 \geq 1$. Let G_0 be a graph obtained by replacing all double edges by a single edge. Note that there are at most $n_1 + n_2$ vertices of degree 1 in G_0. Since G_0 is a tree, it follows that it has at least two leaves, *i.e.*, that $n_1 + n_2 \geq 2$.

It remains to prove that $n_1 = n_3 = 0 \Rightarrow n_2 = 2$. From $n_1 + 2n_2 \geq 4$, it directly follows that $n_2 \geq 2$, so we need to prove that $n_2 \leq 2$.

Suppose the contrary. Let G' $\in \Gamma_{12}$ be a graph with the smallest number of vertices in Γ_{12} without any vertices of degrees 1 and 3 and with at least three vertices of degree 2. Distinguish three cases:

CASE 1: There is a vertex of degree 2 with a single neighbor (connected by a double edge) of degree 2. Since G' is connected, this is graph P_2' (given in Figure 4), but this graph has only two vertices of degree 2, which is a contradiction.

CASE 2: There is a vertex of degree 2 with a single neighbor (connected by a double edge) of degree 4.

Let G'' be a graph obtained by deletion of this vertex of degree 2 and its incident edges. Note that G'' has no vertices of degrees 1 and 3; it has the same number of vertices of degree 2 as G; and it has a smaller number of vertices, which is a contradiction.

CASE 3: Each vertex of degree two has two neighbors.

Note that in this case $e_2(G) \leq n_4 - 1$. We have:

$$2n_2 + 4n_4 = 2(n_2 + n_4 - 1 - e_2(G')) + 4e_2(G')$$
$$2n_2 + 4n_4 \leq 2(n_2 + n_4 - 1 - (n_4 - 1)) + 4(n_4 - 1)$$
$$0 \leq -4,$$

which is a contradiction.

We have exhausted all cases and our theorem is proved. ■

Let us prove some more auxiliary results:

Lemma 10. – Let G $\in \Gamma_{13}$ be a graph with at least one single edge such that υ(G) = (n_1, n_2, n_3, n_4). Then there is a graph G' $\in \Gamma_{13}$ with at least one single edge such that υ(G') = (n_1, n_2, n_3, n_4 + 2).

Proof. Graph G' is obtained from graph G by replacing a single edge with an item depicted below:

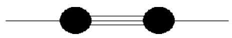

Figure 13. Item that replaces an edge of G.

■

Lemma 11. – Let G $\in \Gamma_{13}$ be a graph such that υ(G) = (n_1, n_2, n_3, n_4) and let $n_1 \geq 1$. Then, there is a graph G' $\in \Gamma_{13}$ such that υ(G') = (n_1 – 1, n_2, n_3 + 1, n_4 + 1).

Proof. Graph G' is obtained from graph G by replacing a leaf and its incident edge:

Figure 14. Leaf and incident edge.

by:

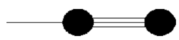

Figure 15. Item that replaces a leaf and incident edge.

■

These Lemmas imply:

Lemma 12. – Let G $\in \Gamma_1$ be a graph such that υ(G) = (n_1, n_2, n_3, n_4), and let $x \leq n_1$, and $y \in N_0$. Then there is a graph G' $\in \Gamma_{13}$ such that $\upsilon(G') = (n_1 - x, n_2, n_3 + x, n_4 + x + 2y)$.

In the paper,[6] the following Lemma is proved:

Lemma 13. – Let $n_1, n_2, n_3, n_4 \in N_0$. Then, there is a graph G $\in \Gamma_1$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ if and only if $n_1 = n_3 + 2n_4 + 2$.

From the last two Lemmas, it follows that:

Lemma 14. – Let $n_1, n_2, n_3, n_4 \in N_0$. If there are numbers $x, y \in N_0$ such that $x + 2y \le n_4$, $x \le n_3$ and $x + y = (n_3 + 2n_4 - n_1 + 2) / 4$. Then, there is a graph G' $\in \Gamma_{13}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$.

Proof. Just note that the last relation is equivalent to

$$n_1 + x = (n_3 - x) + 2(n_4 - x - 2\,y) + 2.$$

■

Now, we can prove our second theorem:

Theorem 15. – Let $n_1, n_2, n_3, n_4 \in N_0$. Then, there is a graph G' $\in \Gamma_{13}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ if and only if $n_1 = n_2 = n_4 = 0$ and $n_3 = 2$, or the following holds:

1) $n_3 + 2n_4 + 2 - n_1 = 0 \pmod 4$

2) $0 \le (n_3 + 2n_4 + 2 - n_1) / 4 \le \min \{(n_3 + n_4) / 2, n_4\}$.

Proof. First, let us prove necessity. If $n_1 = n_2 = n_4 = 0$ and $n_3 = 2$, the claim is trivial, hence suppose that relations 1) and 2) hold. Note that $q = (n_3 + 2n_4 + 2 - n_1) / 4 \in N_0$. We have:

$$\max \{2q - n_4, 0\} \le \min \{n_3, n_4, q\}.$$

Therefore, there exists a natural number x such that

$$\max \{2q - n_4, 0\} \le x \le \min \{n_3, n_4, q\}.$$

Note that $y = q - x \in N_0$ and that

$$x + 2y \le n_4;\ x \le n_3;\ x + y = (n_3 + 2n_4 + 2 - n_1) / 4,$$

hence, by the last Lemma, the graph with the required properties exists.

Now, let us prove sufficiency. If $\upsilon(G) = (0, 0, 2, 0)$ the claim is trivial, so suppose that $\upsilon(G) \ne (0, 0, 2, 0)$. Note that

$$n_1 + 2n_2 + 3n_3 + 4n_4 = \\ 2(n_1 + n_2 + n_3 + n_4 - 1 - e_3(G)) + 6e_3(G);$$

or equivalently that $e_3(G) = q$. Since $e_3(G) \in N_0$, it follows that 1) holds and that $q \ge 0$. Note that each triple edge is incident to at least one of the vertices of degree 4 and that each vertex of degree 4 is incident to at most one triple edge; hence indeed $q \le n_4$. Let G' be a graph obtained from graph G by deleting all its single edges and vertices of degrees 1 and 2 and replacing all triple edges by a single edge. Note that $\Delta(G) \le 1$. We have

$$q = e_3(G) = e(G') \le (\Delta(G') \bullet n(G')) / 2 = (n_3 + n_4) / 2.$$

This proves our claim. ■

Denote by Γ'_{12} the set of graphs in Γ_{12} that have at least one single edge. We need more arbitrary results:

Lemma 16. – Let $n_1, n_2, n_3, n_4 \in N_0$. Then, there is a graph G $\in \Gamma'_{12}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ if and only if $n_2 = n_3 = n_4 = 0$ and $n_1 = 2$; or the following holds:

1) $n_1 \equiv n_3 \pmod 2$

2) $n_1 \le n_3 + 2n_4 + 2$

3) if $n_3 = 0$, then $n_1 + 2n_2 \ge 4$

4) if $n_3 \ge 1$, then $n_1 + n_2 \ge 2$

5) $n_1 + n_3 > 1$.

Proof. Let us prove necessity. If 1) – 5) holds, there is a graph G $\in \Gamma_{12}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ that has at least one vertex of an odd degree. Then there is a single edge incident to this vertex; hence G $\in \Gamma'_{12}$.

Now, let us prove sufficiency. From Theorem 9, it follows that 1) – 4) hold and that either 5) holds or $n_1 = n_3 = 0$ and $n_2 = 2$. Suppose to the contrary that 5) does not hold. Then there is a graph G $\in \Gamma'_{12}$ such that $\upsilon(G) = (0, 2, 0, n_4)$. We have

$$0 + 2 \bullet 2 + 3 \bullet 0 + 4n_4 = \\ 2(0 + 2 + 0 + n_4 - 1 - e_2(G)) + 4e_2(G).$$

Note that $e_2(G) \le v(G) - 1 - 1 \le n_4$, hence

$$4 + 4n_4 \le 2 + 2n_4.$$

This is a contradiction. ■

Lemma 17. – Let $n_1, n_2, n_3, n_4 \in N_0$. There is a graph G $\in \Gamma_{123}$ such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$ if and only if one of the following holds:

1) $n_1 = n_2 = n_4 = 0$ and $n_3 = 2$

2) $n_1 = n_3 = 0$ and $n_2 = 2$

3) there are $x, y \in N_0$ such that $x + 2y \le n_4$, $x \le n_3$ and a graph G' $\in \Gamma'_{12}$ such that $\upsilon(G') = (n_1 + x, n_2, n_3 - x, n_4 - x - 2y)$.

Proof. First, let us prove necessity. If 1) or 2) hold, the claim is trivial. So suppose that 3) holds. Let G'' $\in \Gamma_{123}$ be a graph obtained from graph G' by replacing one of its single edges by:

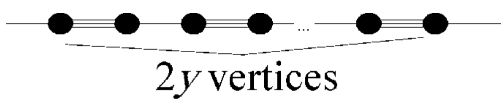

Figure 16. Item that replaces an edge of G'.

Note that $\upsilon(G'') = (n_1 + x, n_2, n_3 - x, n_4 - x)$. Choose arbitrary x leaves in G''. Let G be a graph obtained by replacing each of these vertices (with its incident edge) by an item:

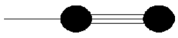

Figure 17. Item that replaces a vertex (with its incident edge) of G''.

Graph G has the required properties.

Now let us prove sufficiency. Let G $\in \Gamma_{123}$ be a graph such that $\upsilon(G) = (n_1, n_2, n_3, n_4)$. If ($n_1 = n_2 = n_4 = 0$ and $n_3 = 2$) or ($n_1 = n_3 = 0$ and $n_2 = 2$), the claim is trivial, so suppose that this is not the case.

Let us prove that G has at least one single edge. Note that each triple edge is incident to at least one vertex of degree four. Hence, there is a single edge or G $\in \Gamma_{12}$. Therefore, there is a single edge or there are no vertices of an odd degree in G, but then $n_1 = n_3 = 0$ and (from Theorem 9) $n_2 = 2$ and we have assumed that this is not the case. Therefore, indeed G has a single edge.

Denote by X the set of all pairs of vertices of degrees 3 and 4 connected by a triple edge and by Y the set of pairs of vertices of degree 4 connected by a triple edge. Also, denote cardinalities of sets X and Y by x = card X and y = card Y. Let G' be a graph obtained by replacing each pair of vertices in X (together with their adjacent edges) by a single edge and by replacing each pair of vertices in Y (together with their adjacent edges) by a single leaf, as shown on the drawing below:

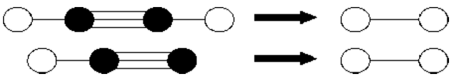

Figure 18. Replacement of graph items.

Note that G' $\in \Gamma'_{12}$ and that $\upsilon(G') = (n_1 + x, n_2, n_3 - x, n_4 - x - 2y)$. ■

It can be easily proved that:

Lemma 18. – Let $n_1, n_2, n_3, n_4 \in N_0$. There are $x, y \in N_0$ such that $x + 2y \le n_4$, $x \le n_3$ and that $n_2 = n_3 - x = n_4 - x - 2y = 0$ and $n_1 = 2$ if and only if

$$n_1 = 2,\ n_2 = 0,\ n_4 \ge n_3 \text{ and } n_4 \equiv n_3 \pmod 2.$$

Let us prove:

Lemma 19. – Let $n_1, n_2, n_3, n_4 \in N_0$. There are $x, y \in N_0$ such that $x + 2y \le n_4$, $x \le n_3$ and that:

1) $n_1 + x \equiv n_3 - x \pmod 2$

2) $n_1 + x \le (n_3 - x) + 2(n_4 - x - 2y) + 2$

3) if $n_3 - x = 0$, then $(n_1 + x) + 2n_2 \ge 4$

4) if $n_3 - x \ge 1$, then $(n_1 + x) + n_2 \ge 2$

5) $(n_1 + x) + (n_3 - x) > 1$

if and only if

I) $n_1 \equiv n_3 \pmod 2$

II) $n_1 \le n_3 + 2n_4 + 2$

III) if $n_3 = 0$, then $n_1 + 2n_2 \ge 4$

IV) if $n_3 \ge 1$, then $n_1 + n_2 \ge \max\{2 - n_4, 3 - n_3, 2 - (n_3 + 2n_4 + 2 - n_1) / 4\}$

V) $n_1 + n_3 > 1$.

Proof: First, let us prove sufficiency. Relations 1) and 5) are equivalent to I) and V). Relation 2) is equivalent to $n_1 + 4x + 2y \le n_3 + 2n_4 + 2$, which implies II). Distinguish two cases:

CASE 1: $n_3 = 0$.

Relation IV) is trivial. Note that $x = 0$, hence III) holds.

CASE 2: $n_3 \ge 1$.

Relation III) is trivial. It remains to prove IV). Suppose that relation 1) – 5) hold for $x = n_3$. Note that in this case these relations also hold for $x = n_3 - 1$. Suppose that relation 1) – 5) hold for $y \in N_0$. Note that in this case they also hold for $y = 0$. Therefore, we may assume that $x \le n_3 - 1$ and $y = 0$. Relations 2) and 4) can be rewritten as

$$x \le (n_3 + 2n_4 + 2 - n_1) / 4$$
$$x \ge 2 - n_1 - n_2$$

Combining this with $x \ge 0$; $x \le n_3 - 1$ and $x \le n_4$, we get

$$2 - n_1 - n_2 \le (n_3 + 2n_4 + 2 - n_1) / 4$$
$$2 - n_1 - n_2 \le n_3 - 1$$
$$2 - n_1 - n_2 \le n_4.$$

From these relations, IV) easily follows.

Now, let us prove necessity. Relations 1) and 5) are equivalent to I) and V). Distinguish two cases:

CASE 1: $n_3 = 0$.

It is sufficient to take $x = y = 0$.

CASE 2: $n_3 \ge 1$.

Note that

$$\max\{0, 2 - n_1 - n_2\} \le \min\{(n_3 + 2n_4 + 2 - n_1) / 4, n_3 - 1, n_4\}.$$

Hence, there is an integer x such that

$$\max\{0, 2 - n_1 - n_2\} \le x \le \min\{(n_3 + 2n_4 + 2 - n_1) / 4, n_3 - 1, n_4\}.$$

Taking $y = 0$ and this x, the claim follows. ■

From the last four Lemmas, our third theorem follows directly:

Theorem 20. – Let $n_1, n_2, n_3, n_4 \in N_0$. There is a graph G $\in \Gamma_{123}$ if and only if one of the following holds:

1) $n_1 = n_2 = n_4 = 0$ and $n_3 = 2$

2) $n_1 = n_3 = 0$ and $n_2 = 2$

3) $n_1 = 2$, $n_2 = 0$, $n_4 \geq n_3$ and $n_4 \equiv n_3 \pmod 2$

4) The following five relations hold:

4.1) $n_1 \equiv n_3 \pmod 2$

4.2) $n_1 \leq n_3 + 2n_4 + 2$

4.3) if $n_3 = 0$, then $n_1 + 2n_2 \geq 4$

4.4) if $n_3 \geq 1$, then $n_1 + n_2 \geq \max \{2 - n_4, 3 - n_3, 2 - (n_3 + 2n_4 + 2 - n_1) / 4\}$

4.5) $n_1 + n_3 > 1$.

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. We determine here the necessary and sufficient conditions of 4-tuples (n_1, n_2, n_3, n_4) for the existence of a graph G such that G has n_1, n_2, n_3 and n_4 vertices of degrees 1, 2, 3 and 4. Some results for graphs having only single edges have been already discussed in literature, but here we have proved three theorems that cover graphs with single and/or double edges, with single and/or triple edges, and with single and/or double and/or triple edges, respectively. This results further the results given in Kier *et al.*[8] and Skvortsova *et al.*[9]

As degree sequences (or equivalently 4-tuples) have already served to define a number of topological indices[7] able to correlate molecular properties,[10] the results achieved here could be of interest when one is interested to take into account multiple covalent bonds in molecules.

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SAŽETAK

Kompaktni slijedovi valencija za molekule s jednostrukim, dvostrukim i trostrukim vezama

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Molekularni grafovi zvani plerografovi mogu modelirati višestruke veze u molekulama. U ovom radu su definirani kompaktni slijedovi valencija plerografova. Dokazana su tri teorema koji daju nužne i dovoljne uvjete da bi zadani slijed opisivao neki plerograf.