Journal of Mathematical Chemistry 11(1992)353–364

AN EXISTENCE THEOREM FOR MOLECULAR GRAPHS DETERMINED BY A SEQUENCE OF VALENCE STATES

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Received 1 October 1991

Abstract

Vertices of molecular graphs (multigraphs with restricted vertex valences and edge multiplicities) are described by the so-called valence states – an ordered triple of non-negative integers that are equal to the number of edges with a given multiplicity that are incident with the vertex. For molecular graphs, which correspond to standard organic-chemistry compounds composed of H, C, N, and O atoms, there may appear only ten eligible valence states. In order to construct exhaustively all graphs assigned to a given sequence of valence states, it is advantageous to know under what condition the sequence is graphical. An existence theorem for sequences composed of eligible valence states to be graphical is proved.

1. Introduction

The problem of constructive enumeration of molecular graphs belongs to the interesting problems of mathematical chemistry. It is very important not only for computer-assisted structure elucidation [1,2], but also for computer-assisted synthesis design [3] and for verifications (or falsifications) of hypotheses concerning a relation between "topology" of molecular graphs and their properties [4,5].

Many effective methods for constructive enumeration have been elaborated and implemented on computers. One main problem in these techniques is the way of specification of the molecular graphs to be constructed. The simplest one is to specify the molecular graphs by the number of vertices and edges. Although this approach is very simple and straightforward, it neglects many structural details of graphs.

In computer-assisted structure elucidation, another possible way is used for determining graphs, in which they are prescribed not only by the number of vertices but also by some subgraphs – molecular fragments – that have (not) to appear in constructed graphs [1]. This approach leads naturally to the technique of the so-called superatoms (supervertices) [1] that are in the final stage of constructive enumeration expanded to given subgraphs. The role of automorphism of prescribed subgraphs is usually ignored and the redundancy of resulting graphs is checked in the final stage of enumeration. A possible way of avoiding these and other similar problems is to determine the molecular graphs by a prescribed sequence of valence states [6,7]. The main superiority of this method lies in the fact that valence states of vertices correspond to the simplest "fragments" with transparent chemical interpretation.

Another interesting possibility to use the sequence of valence states is in the field of a reconstruction problem of topological indices [8]. The approach of topological indices belongs in mathematical chemistry to quite popular techniques used for the study of correlations between molecular graphs and their properties. Therefore, it seems that an inverse problem – to construct all graphs with the value of a given topological index from a prescribed interval – might be of interest for the prediction of molecular graphs endowed by a required property. Gordeeva and Zefirov [5] have attacked this reconstruction problem for the Randić topological indices [9]. The authors produced in an initial stage all sequences of valence states that may potentially give a required value of the index, and then an attempt is made to construct all graphs corresponding to the produced sequences.

Conditions in computer-assisted structure elucidation due to data of some type of spectroscopy may be satisfied by several sequences of valence states of atoms. This is also true for some ranges of topological index values. It is not always certain whether there can exist molecular graphs composed of given atoms in prescribed valence states. As an example can serve a sequence of one four-valence carbon, one three-valence nitrogen, and three one-valence hydrogens. One may simply verify that there should not exist molecular graphs without multiple bonds containing only these atoms in given valence states. This means that when we are constructing molecular graphs composed of atoms in required valence states, it is vitally important to know the negative cases (non-graphical) in advance. For these cases we can omit the construction, which may be time-consuming even if it did not produce any molecular graphs.

The purpose of this communication is to prove an existence theorem for sequences of eligible valence states to be graphical. The necessary and sufficient condition under which a sequence of valence states is graphical is formulated, i.e. a condition stating whether there exists a multigraph with the same sequence as that prescribed. If this condition is satisfied, a constructive enumeration of molecular graphs with a prescribed sequence of eligible valence states should provide a non-empty list of constructed graphs.

2. Sequences of valence states

Let G be the so-called *molecular graph* determined as a *multigraph* [10,11] with a non-empty *vertex set* $V(G)$ and an *edge set* $E(G)$. A *multiplicity* of an edge $e \in E(G)$ is denoted by mul(e). The notion of multiplicity may be extended outside $E(G)$; we then say an edge $e \notin E(G)$ is of zero multiplicity. A *valence* of a vertex $\upsilon \in V(G)$, val(υ), is a non-negative integer determined as a sum of multiplicities of all edges incident with the vertex. Finally, we shall always assume that the molecular graph G *contains at most triple edges and vertex valences, that are bounded from above by 4.* A vertex with zero valence corresponds to an isolated vertex. These requirements considerably restrict the notion of molecular graphs, now it is closely related to the usual meaning of structural formulae in organic chemistry.

A *valence state* [6,12,13] of a vertex $v \in V(G)$ is determined as an ordered triple of non-negative integers, $\mathrm{vs}(v) = (n_1, n_2, n_3)$, where the entry n_i (for $1 \le i \le 3$) is equal to the number of i-tuple edges incident with the vertex v. Using these entries, a valence assigned to the vertex v is determined by $\mathrm{val}(v) = n_1 + 2n_2 + 3n_3$. Since the valences are bounded from above by 4, entries of valence states cannot be arbitrary non-negative integers, they are restricted by $0 \le n_1 + 2n_2 + 3n_3 \le 4$. Solving this inequality for non-negative integers, we arrive at ten valence states, called the *eligible valence states*, displayed in fig. 1.

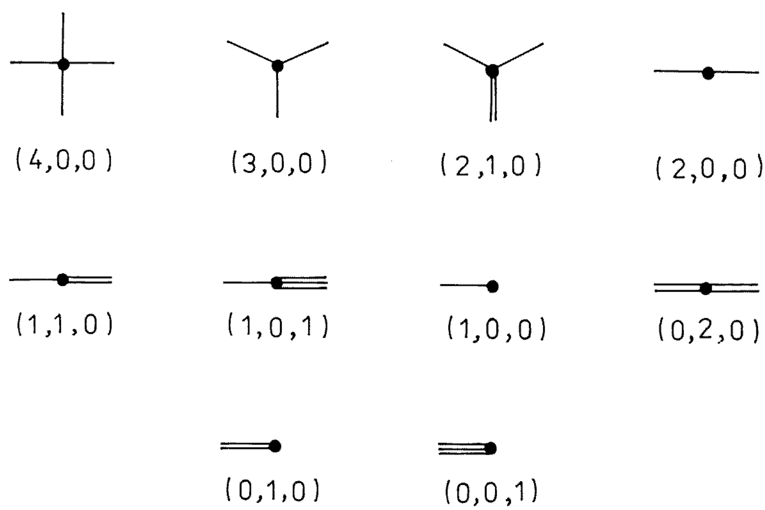

Fig. 1. All possible eligible valence states that may appear in molecular graphs. Below each graphical representation of valence states, an ordered triple of non-negative integers is presented.

Let Ξ be a sequence of p eligible valence states

$$\Xi = (\mathrm{vs}_1, \mathrm{vs}_2, \ldots, \mathrm{vs}_p); \tag{1}$$

it will be called *graphical* if there exists a multigraph, composed of p vertices, with the same sequence of valence states, $\mathrm{seq}(G) = \Xi$. If we would like to construct all multigraphs with the prescribed sequence of valence states, then it is important to know, in advance, whether this sequence is graphical. In other words, if a sequence $\Xi = (\mathrm{vs}_1, \mathrm{vs}_2, \ldots, \mathrm{vs}_p)$ is given, then under what condition does a sequence Ξ correspond to a multigraph?

We shall study a simpler problem. Let G be a simple graph (without multi-edges) composed of p vertices and q edges. Let its sequence of vertex valences be denoted by

$$\mathrm{seq}(G) = \Pi = (\mathrm{val}_1, \mathrm{val}_2, \ldots, \mathrm{val}_p), \tag{2a}$$

where [10, 11]

$$\sum_{i=1}^{p} \mathrm{val}_i = 2q. \tag{2b}$$

A necessary and sufficient condition for a sequence (2a) to be graphical was found by Havel [14] and Hakimi [15] (cf. also refs. [10, 11]).

THEOREM 1

A sequence $\Pi = (\mathrm{val}_1, \mathrm{val}_2, \ldots, \mathrm{val}_p)$ of non-negative integers with $\mathrm{val}_1 \geq \mathrm{val}_2 \geq \ldots \geq \mathrm{val}_p$, where $\mathrm{val}_1 \leq p-1$ and $p \geq 2$, is graphical if and only if the sequence $\Pi' = (\mathrm{val}_2 - 1, \mathrm{val}_3 - 1, \ldots, \mathrm{val}_{\mathrm{val}_1+1} - 1, \mathrm{val}_{\mathrm{val}_1+2}, \ldots, \mathrm{val}_p)$ is graphical.

This theorem allows us to suggest a very simple recurrent algorithm for checking whether a sequence of non-negative integers is graphical [11].

We now return to our original problem, namely to find a necessary and sufficient condition for sequence (1) to be graphical. Let us construct from sequence (1) five sequences of p non-negative integers:

$$\Pi_i = (n_i^{(1)}, n_i^{(2)}, \ldots, n_i^{(p)}) \qquad (\text{for } i = 1,2,3), \tag{3a}$$

$$\Pi_{12} = (n_1^{(1)} + n_2^{(1)}, n_1^{(2)} + n_2^{(2)}, \ldots, n_1^{(p)} + n_2^{(p)}), \tag{3b}$$

$$\Pi_{13} = (n_1^{(1)} + n_3^{(1)}, n_1^{(2)} + n_3^{(2)}, \ldots, n_1^{(p)} + n_3^{(p)}). \tag{3c}$$

Sequence Π_i was formed from the ith entries of valence states of the sequence Ξ; sequence Π_{12} (Π_{13}) is composed of entries that are equal to the sum of 1st and 2nd (3rd) entries in valence states of Ξ; formally, we may write $\Pi_{12} = \Pi_1 + \Pi_2$ ($\Pi_{13} = \Pi_1 + \Pi_3$).

THEOREM 2

A sequence $\Xi = (\mathrm{vs}_1, \mathrm{vs}_2, \ldots, \mathrm{vs}_p)$ composed of eligible valence states is graphical if and only if all sequences Π_1, Π_2, Π_{12}, and Π_{13} are graphical.

According to this theorem, a verification whether the sequence $\Xi = (\mathrm{vs}_1, \mathrm{vs}_2, \ldots, \mathrm{vs}_p)$ is graphical may be done by applying separately the algorithm suggested with the aid of theorem 1 [11] to all four sequences Π. If in this process some of them are not graphical, then the sequence Ξ is not graphical either.

Example 1

An application of theorem 2 is illustrated by the sequence composed of six eligible valence states,

$$\Xi = ((2, 1, 0), (2, 1, 0), (1, 0, 1), (1, 0, 1), (1, 0, 0), (1, 0, 0)).$$

From this sequence of valence states, we form five sequences (see eqs. (3a)–(3c)):

$$\Pi_1 = (2, 2, 1, 1, 1, 1),$$

$$\Pi_2 = (1, 1, 0, 0, 0, 0),$$

$$\Pi_3 = (0, 0, 1, 1, 0, 0),$$

$$\Pi_{12} = \Pi_1 + \Pi_2 = (3, 3, 1, 1, 1, 1),$$

$$\Pi_{13} = \Pi_1 + \Pi_3 = (2, 2, 2, 2, 1, 1).$$

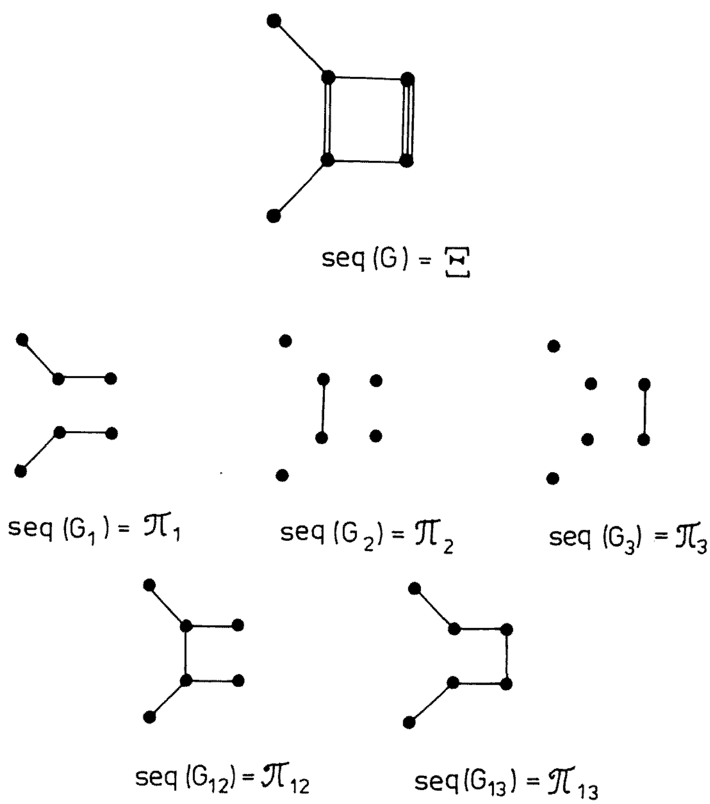

Fig. 2. An example of multigraph G assigned to the sequence Ξ specified in example 1; corresponding graphs $G_1, G_2, \ldots, G_{13}$ assigned to sequences $\Pi_1, \Pi_2, \ldots, \Pi_{13}$ (see example 1), respectively, are given in the lower part of the figure.

Applying the algorithm given in ref. [11], we verify that sequences Π_1, Π_2, Π_{12}, and Π_{13} are graphical; hence, from theorem 2, the sequence Ξ is graphical. An example of a multigraph with the sequence of valence states Ξ and the corresponding simple graphs assigned to sequences Π is shown in fig. 2.

3. Proof of theorem 2

3.1. NECESSARY CONDITION

Let us assume that the sequence Ξ is graphical, then there exists a multigraph with the sequence of valence states equal to Ξ, i.e. seq(G) = Ξ. From the multigraph G, we may unambiguously construct the following five simple graphs (without multi-edges). Graph G_i (for $i = 1, 2, 3$) is created from G by deleting all edges with multiplicity other than i and the remaining multi-edges (if any) are substituted by single edges. Valence sequences of these three graphs G_1, G_2, and G_3 are equal to the sequences Π_1, Π_2, and Π_3, respectively. A graph G_{12} (G_{13}) is created from the multigraph G by deleting all triple (double) edges, and double (triple) edges (if any) are substituted by single edges; a valence sequence of this graph is equal to $\Pi_{12} = \Pi_1 + \Pi_2$ ($\Pi_{13} = \Pi_1 + \Pi_3$), see fig. 2. Consequently, since the graphs G_1, G_2, G_3, G_{12}, and G_{13} (unambiguously constructed from the multigraph G) have valence sequences Π_1, Π_2, Π_3, Π_{12}, and Π_{13}, respectively, these sequences are graphical.

3.2. SUFFICIENT CONDITION

Let us assume that the sequence Π_1 is graphical, i.e. there exists a graph G such that seq(G) = Π_1. Assuming that the sequence Π_2 is also graphical, then the graph G may be enlarged so that, according to Π_2, double edges are introduced. When adding the double edges, the already placed single edges will not be considered as restraining, only the cases with non-eligible valence states are expelled. What we have to discuss now is a potential simultaneous appearance of single and double edges between pairs of vertices in G; such graphs will be called *intruder graphs*. Since the sequences Π_1 and Π_2 correspond to a sequence composed of eligible valence states only, we demonstrate that some part of them may be simply transformed to non-intruder graphs (with sequences Π_1 and Π_2) and the remaining ones (which could not be transformed to a non-intruder form) are rejected from our considerations by the assumption that the sequence Π_{12} is graphical. The intruder graphs with graphical sequences Π_1 and Π_2 are displayed in a schematic form in fig. 3. For eligible valence states, there exist three different cases in which a pair of vertices is adjacent simultaneously by single and double edges. Since sequences Π_{12} assigned to "minimal" subgraphs induced by vertices lying over boxes in fig. 3 as well as by vertices that are adjacent with the previous ones, i.e. (2, 2), (3, 2, 1), (3, 3, 1, 1), and (3, 3, 2), are not graphical, there must exist other edges inside the box. When considering some new edges in the box, these schemes may produce three intruder graphs with non-graphical sequences Π_{12}, see fig. 4. All other possibilities produced

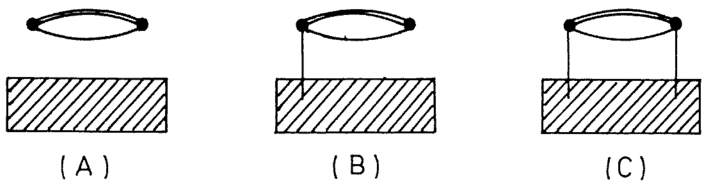

Fig. 3. Three schematic forms of intruder graphs in which a pair of vertices is adjacent simultaneously by single and double edges. The sequences Π_1 and Π_2 assigned to these graphs are graphical. Shadowed rectangular blocks represent rests of graphs.

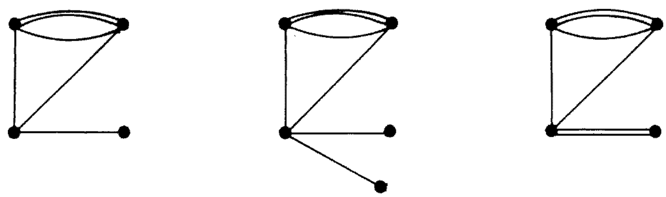

Fig. 4. Intruder graphs derived from scheme C in fig. 3. For all these graphs, the sequence Π_{12} is non-graphical.

by these schemes can be transformed by an approach (initially used by Havel [14] in his proof of theorem 1) to a form of standard multigraphs composed of single and double edges. Let us assume that vertices v_i and v_j are adjacent simultaneously by single and double edges. Then there exists a single or double edge (taken from the box) adjacent with other vertices v_k and v_l such that pairs of vertices v_i, v_k and v_j, v_l are not adjacent in G. The graph G is transformed into another graph by deleting the edges (v_i, v_j) and (v_k, v_l) and creating new edges (v_i, v_k) and (v_j, v_l). The resulting graph has the same valence sequences Π_1 and Π_2 as the original one, the vertices v_i and v_j are adjacent either by a single or double edge but not both of them, see fig. 5. Repeating the above procedure for all cases in which single and

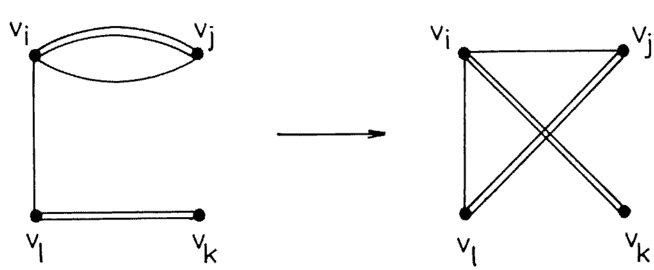

Fig. 5. An illustrative example of Havel's procedure of removing edges (v_i, v_j) and (v_k, v_l) and creating new edges (v_i, v_k) and (v_j, v_l), where the initial and produced graphs have the same sequences Π_1 and Π_2.

double edges are simultaneously incident with pairs of vertices, we arrive at a non-intruder multigraph G composed of single and double edges and with sequences Π_1 and Π_2.

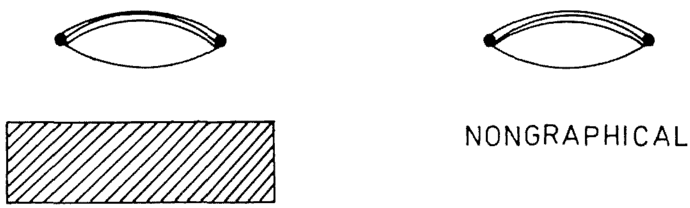

Fig. 6. Schematic form of intruder graphs in which a pair of vertices is adjacent simultaneously by single and triple edges. The shadowed block represents a component of an intruder graph; if this block is an empty graph, then a sequence Π_{13} of this intruder graph is non-graphical.

The only form of intruder graphs allowed for eligible valence states, when triple edges are allowed (determined by a graphical sequence Π_3), is displayed in fig. 6. For this case, an analogous approach as for single and double edges is applicable, transforming an intruder graph in a proper multigraph with sequences Π_1, Π_2, and Π_3.

A sequence Π_3 may be composed only from entries "1", that means any such sequence which has the sum of its members equal to an even number is graphical. Since the sequences Π_1 and Π_{13} are graphical, they must also have an even sum of their members. Since $\Pi_3 = \Pi_{13} - \Pi_1$, the sum of members of Π_3 must also be even. Therefore, if Π_1 and Π_{13} are graphical, then Π_3 must also be graphical. In summary, we have proved that, if sequences Π_1, Π_2, Π_{12}, and Π_{13} are graphical, then there exists a multigraph G with $\mathrm{seq}(G) = \Xi = (\Pi_1, \Pi_2, \Pi_3)$. □

We would like to emphasize that theorem 2 cannot be generalized for multigraphs composed of other valence states than eligible ones. Its proof is based on the assumption that the used valence states are eligible. For instance, let us consider a sequence $\Xi = ((3, 1, 0), (2, 0, 0), (2, 0, 0), (1, 2, 0), (0, 1, 0))$, where the first and fourth valence states are not eligible. Although sequences $\Pi_1 = (3, 2, 2, 1, 0)$, $\Pi_2 = (1, 0, 0, 2, 1)$ and $\Pi_{12} = (4, 2, 2, 3, 1)$ are graphical (a sequence Π_{13} should not be considered, the sequence Ξ does not contain triple edges), it is impossible to construct a multigraph which corresponds to Ξ, see fig. 7. It seems that theorem 2 remains valid if the set of eligible valence states is enlarged by further valence states containing only single edges or only double or triple edges. While these added valence states do not change the scheme of our proof of theorem 2, we have to be very careful when the set of eligible valence states is enlarged by valence states with mixed multiplicities of edges. For instance, as follows from the above illustrative example, valence states $(3, 1, 0)$ and $(1, 2, 0)$ may cause a failure of theorem 2.

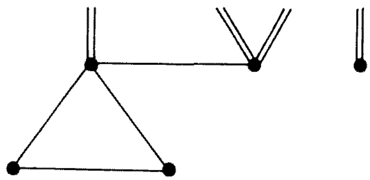

Fig. 7. An illustrative example of non-graphical sequence Ξ = ((3, 1, 0), (2, 0, 0), (2, 0, 0), (1, 2, 0), (0, 1, 0)) with graphical sequences Π_1, Π_2, Π_{12}.

4. Applications

Theorem 2 offers a simple way to construct all possible sequences of eligible valence states for multigraphs with a prescribed number of vertices and single, double, and triple edges. If we have to enumerate molecular graphs specified by, for instance, the number of atoms, rings and multiple bonds, we generate all possible sequences of valence states corresponding to this specification. The resulting sequences are proper objects for determination of molecular graphs that have to be constructively enumerated.

An algorithm for generation of all possible sequences of eligible valence states can be easily implemented in a backtrack form. In tables 1–4 are given illustrative results for multigraphs composed of six vertices and a prescribed number of single, double, and triple edges.

We have to emphasize that we may produce sequences of valence states that are graphical but realized by disconnected multigraphs only. For instance, a sequence $\Xi = ((2, 0, 0)^3(0, 2, 0)^3)$ is obviously graphical but its only realization corresponds to a disconnected multigraph with two triangular components, which are composed of single and double edges, respectively. Graph-theoretically [10, 11], the number of vertices (p), edges (q), cycles (c), and components (n) are mutually related by $c = q - p + n$; that is, fixing its two entries (e.g. p and q), we have only one restrictive condition for the remaining two entries (e.g. c and n). This means there may exist several feasible solutions of the above condition.

For our illustrative example of multigraphs, composed of six vertices, three single edges and three double edges, we obtain two feasible solutions, $c = 1$, $n = 1$ and $c = 2$, $n = 2$, where the second solution can be realized by the triangles mentioned above. Summarizing our considerations, we may say that it is impossible to decide in advance whether a graphical sequence of valence states is realized by disconnected graphs only.

Fortunately, many of such sequences are removed from our considerations by necessary conditions that are satisfied for disconnected multigraphs only. In particular, if entries of a given sequence may be separated into two or more disjoint classes that are composed either of valence states with single, or double, or triple, or single and double edges in one class and triple edges in the other class, etc., then this

Table 1

All possible graphical sequences of eligible valence states corresponding to six vertices and six single edges.

No.	Sequence
1	$(4, 0, 0)^1$ $(3, 0, 0)^1$ $(2, 0, 0)^1$ $(1, 0, 0)^3$
2	$(4, 0, 0)^1$ $(2, 0, 0)^3$ $(1, 0, 0)^2$
3	$(3, 0, 0)^1$ $(2, 0, 0)^4$ $(1, 0, 0)^1$
4	$(3, 0, 0)^2$ $(2, 0, 0)^2$ $(1, 0, 0)^2$
5	$(3, 0, 0)^3$ $(1, 0, 0)^3$
6	$(2, 0, 0)^6$

Table 2

All possible graphical sequences of eligible valence states corresponding to six vertices, five single edges, and one double edge.

No.	Sequence
1	$(4, 0, 0)^1$ $(2, 1, 0)^1$ $(2, 0, 0)^1$ $(1, 0, 0)^2$ $(0, 1, 0)^1$
2	$(4, 0, 0)^1$ $(2, 1, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 0)^3$
3	$(4, 0, 0)^1$ $(2, 0, 0)^1$ $(1, 1, 0)^2$ $(1, 0, 0)^2$
4	$(4, 0, 0)^1$ $(2, 0, 0)^2$ $(1, 1, 0)^1$ $(1, 0, 0)^1$ $(0, 1, 0)^1$
5	$(3, 0, 0)^1$ $(2, 1, 0)^1$ $(2, 0, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 0)^2$
6	$(3, 0, 0)^1$ $(2, 1, 0)^1$ $(2, 0, 0)^2$ $(1, 0, 0)^1$ $(0, 1, 0)^1$
7	$(3, 0, 0)^1$ $(2, 1, 0)^2$ $(1, 0, 0)^3$
8	$(3, 0, 0)^1$ $(2, 0, 0)^2$ $(1, 1, 0)^2$ $(1, 0, 0)^1$
9	$(3, 0, 0)^1$ $(2, 0, 0)^3$ $(1, 1, 0)^1$ $(0, 1, 0)^1$
10	$(3, 0, 0)^2$ $(2, 1, 0)^1$ $(1, 0, 0)^2$ $(0, 1, 0)^1$
11	$(3, 0, 0)^2$ $(2, 0, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 0)^1$ $(0, 1, 0)^1$
12	$(3, 0, 0)^2$ $(1, 1, 0)^2$ $(1, 0, 0)^2$
13	$(2, 1, 0)^1$ $(2, 0, 0)^3$ $(1, 1, 0)^1$ $(1, 0, 0)^1$
14	$(2, 1, 0)^1$ $(2, 0, 0)^4$ $(0, 1, 0)^1$
15	$(2, 1, 0)^2$ $(2, 0, 0)^2$ $(1, 0, 0)^2$
16	$(2, 0, 0)^4$ $(1, 1, 0)^2$

Table 3

All possible graphical sequences of eligible valence states corresponding to six vertices, four single edges, one double edge, and one triple edge.

No.	Sequence
1	$(4, 0, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 1)^2$ $(1, 0, 0)^1$ $(0, 1, 0)^1$
2	$(4, 0, 0)^1$ $(1, 1, 0)^2$ $(1, 0, 1)^1$ $(1, 0, 0)^1$ $(0, 0, 1)^1$
3	$(3, 0, 0)^1$ $(2, 1, 0)^1$ $(2, 0, 0)^1$ $(1, 0, 1)^1$ $(0, 1, 0)^1$ $(0, 1, 0)^1$
4	$(3, 0, 0)^1$ $(2, 1, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 1)^1$ $(1, 0, 0)^1$ $(0, 0, 1)^1$
5	$(3, 0, 0)^1$ $(2, 1, 0)^1$ $(1, 0, 1)^2$ $(1, 0, 0)^1$ $(0, 1, 0)^1$
6	$(3, 0, 0)^1$ $(2, 0, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 1)^2$ $(0, 1, 0)^1$
7	$(3, 0, 0)^1$ $(2, 0, 0)^1$ $(1, 0, 0)^2$ $(1, 0, 1)^1$ $(0, 0, 1)^1$
8	$(3, 0, 0)^1$ $(1, 1, 0)^2$ $(1, 0, 1)^2$ $(1, 0, 0)^1$
9	$(2, 1, 0)^1$ $(2, 0, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 1)^2$ $(1, 0, 0)^1$
10	$(2, 1, 0)^1$ $(2, 0, 0)^2$ $(1, 1, 0)^1$ $(1, 0, 1)^1$ $(0, 0, 1)^1$
11	$(2, 1, 0)^1$ $(2, 0, 0)^2$ $(1, 0, 1)^2$ $(0, 1, 0)^1$
12	$(2, 1, 0)^2$ $(2, 0, 0)^1$ $(1, 0, 1)^1$ $(1, 0, 0)^1$ $(0, 0, 1)^1$
13	$(2, 1, 0)^2$ $(1, 0, 1)^2$ $(1, 0, 0)^2$
14	$(2, 0, 0)^2$ $(1, 1, 0)^2$ $(1, 0, 1)^2$

Table 4

All possible graphical sequences of eligible valence states corresponding to six vertices, three single edges, and three double edges.

No.	Sequence
1	$(3, 0, 0)^1$ $(1, 1, 0)^2$ $(1, 0, 1)^1$ $(0, 2, 0)^2$
2	$(3, 0, 0)^1$ $(1, 1, 0)^3$ $(0, 2, 0)^1$ $(0, 1, 0)^1$
3	$(2, 1, 0)^1$ $(2, 0, 0)^1$ $(1, 1, 0)^1$ $(1, 0, 0)^1$ $(0, 2, 0)^2$
4	$(2, 1, 0)^1$ $(2, 0, 0)^1$ $(1, 1, 0)^2$ $(0, 2, 0)^1$ $(0, 1, 0)^1$
5	$(2, 1, 0)^1$ $(2, 0, 0)^2$ $(0, 2, 0)^2$ $(0, 1, 0)^1$
6	$(2, 1, 0)^1$ $(1, 1, 0)^3$ $(1, 0, 0)^1$ $(0, 2, 0)^1$
7	$(2, 1, 0)^1$ $(1, 1, 0)^4$ $(0, 1, 0)^1$
8	$(2, 1, 0)^2$ $(2, 0, 0)^1$ $(0, 2, 0)^1$ $(0, 1, 0)^2$
9	$(2, 1, 0)^2$ $(1, 1, 0)^1$ $(1, 0, 0)^1$ $(0, 2, 0)^1$ $(0, 1, 0)^1$
10	$(2, 1, 0)^2$ $(1, 1, 0)^2$ $(0, 1, 0)^2$
11	$(2, 1, 0)^2$ $(1, 0, 0)^2$ $(0, 2, 0)^2$
12	$(2, 1, 0)^3$ $(0, 1, 0)^3$
13	$(2, 0, 0)^1$ $(1, 1, 0)^4$ $(0, 2, 0)^1$
14	$(2, 0, 0)^2$ $(1, 1, 0)^2$ $(0, 2, 0)^2$
15	$(1, 1, 0)^6$

sequence corresponds to multigraphs with the number of components greater than or equal to the number of classes. The above example of sequence $\Xi = ((2,0,0)^3(0,2,0)^3)$ has two classes of valence states, i.e. multigraphs assigned to this sequence are disconnected with two components. In tables 1–4 are given only those sequences that are realized at least by one connected multigraph.

Acknowledgement

The authors gratefully acknowledge comments and suggestions by Dr. L. Šoltés.

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