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METRIC ANALYSIS OF GRAPHS

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A B S T R A C T

In the work presented here the metric properties of graphs are studied. For a graph the relative partitions are introduced and on this basis the graph layer matrix of the order n is defined (at n = 1 the graph layer matrix coincides with a distance degree sequence), which is a basis for the calculation of various characteristics of a graph. For studying the path properties the path layer matrix of a graph is defined (or the path degree sequence). The concept of the graph isotopicity is introduced and the graph isotopicity criterion is given. The properties of a vertex set whose deletion does not influence the metric properties of the remaining vertices are considered.

A study of metric properties of graphs and their use in the chemical research is an important direction in applications of mathematics in chemistry. Metric properties provide the wide possibilities for describing structural features of molecular graphs. Widely known are the topological molecular indices [1] which are used in the studies of the problem for establishing the "structure-property" relationship. A formal representation of metric properties in the form of either indices or other characteristics can also be useful in the field of sciences adjacent to chemistry. At present, one can not say that there is either general approach or a theory for defining or calculating the topological characteristics of molecular structures. A theory of graphs enables one to carry out a systematic study of fundamental properties of graphs and also to consider a set of structural characteristics, the use of which will facilitate the development of a more substantiated system for the description of the structural properties of molecules.

In the work presented here some problems of metric analysis of graphs are considered. The metric analysis of graphs is assumed to be a combination of the methods, algorithms and their computer realization.These mathematical means are used for investigation of various problems as a study of metric properties of graphs, the construction of molecular topological indices, a study of variations in values of indices at local transformations in the molecule structure, defining ways of evaluation of the relative position of fragments in the molecule, etc. In addition, the metric properties of graphs are used for accelerating the calculations in the solutions of such complicated problems as, for example, finding the maximal common parts in graphs, etc. One should note that together with the natural metric of graph based on a distance as the shortest path connecting a pair of verticies , and search for other approaches for the definition of the graphs distances that will enable one to investigate important notions of the similarity in molecular structures The graph properties based on the distance and path distance between the graph verticies are considered here. The metric properties of graphs are based on the notions of the relative partition and graph layer matrix [2] . In particular, in terms of layer matrix the condition of graph isometricity is formed [7] . Also consi -

dered are the use of metric characteristics for defining the relative positions of subgraphs in a graph, a set of vertices of graph is described whose deletion does not change the distances between the remaining vertices.

The work presented here contains a review and some original results obtained at the Institute of Mathematics of the Siberian Division of the USSR Academy of Sciences, Novosibirsk. For the sake of the work unity the references are given and other results are mentioned as considered appropriate. It is worth to note that the work is not an exhaustive review of the studies performed in the field of the graph metric properties. Its main purpose is to make the readers aquainted with some problems of the graphs metric analysis.

I. RELATIVE PARTITION AND GRAPH LAYER MATRIX

Let $G(V,X)$ be the finite undirected connected graph without loops and multiple edges, $V(G)$ is the vertex set of the graph G, $|V(G)|=p$, $|X(G)|=q$. The distance $d(u,v)$ between vertices $u,v \in V(G)$ is assumed to be the length of the shortest path connecting u and v. If $V_0 \subseteq V(G)$, then a distance between $v \in V(G)$ and a set V_0 is a minimal distance between v and vertices from V_0 in graph G. Let $V_i(V_0)$ be a set of vertices of graph G located at a distance i from V_0.

DEFINITION 1 [2]. A relative partition of graph G with respect to $V_0 \subseteq V(G)$ is called an ordered partition

$$\hat{G}(V_0)=\{V_j(V_0) \mid j=0,1,2,\dots,K(V_0), v\in V_j(V_0) \Leftrightarrow d(v,V_0)=j\},\ V_i \cap V_j = \emptyset$$

with $i \neq j$. A set of vertices $V_i(V_0)$ will be called an i-th layer of partition and $K(V_0)$ as a length of partition.

Fig. 1 shows a relative partition of the graph G with respect to $V_0=\{u,v\}$. Let us consider a set of all the relative partitions of the graph G with respect to the subsets $V(G)$ of the order n using these partitions one should put into correspondence of the graph G the layer matrix of the order of n .

DEFINITION 2 [2]. As a layer matrix of the order n of the graph G is called a matrix $\lambda^n(G)=\|\lambda_{ij}\|$, $i=1,2,\dots,\binom{p}{n}$, $j=1,2,\dots,d(G)$, where λ_{ij} is equal to the number of vertices in the j -th layer of a relative partition with respect to the i -th set of the order n, $d(G)$ is a diameter of graph G .

By ordering the lines $\lambda^n(G)$ with the decrease of a length (the number of nonzeroth elements) and then by lexicographic ordering the lines of the same length one can obtain a canonic layer matrix $\lambda^n(G)$. With n = 1 one can obtain a layer matrix $\lambda(G)$ for the single vertex partition of graph G . For further use we take that $\lambda(G)$ has always its canonic form. In the analogy of the vertex layer matrix $\lambda^n(G)$ one can consider an edge layer matrix $\lambda^n_X(G)$ where the j -th component in a line corresponding to some relative partition is a value of the cut between the layers V_{j-1} and V_j of this partition that is equal to the number of edges between the layers V_{j-1} and V_j . The complete graph layer matrix is represented in the form $\lambda^n(V,X)=(\lambda^n(G),\lambda^n_X(G))$. Fig. 2 shows the matrices $\lambda(G)$ and $\lambda_X(G)$ of graph G .

Let the layer matrices be represented in the linear form. For the graph in Fig. 2 $\lambda(G)=\|1(2,1,1);\ 2(1,2,1);\ 3,4,5(3,1,0)\|$. or if the vertex numbers are not necessary, a multiplicity of the similar lines is only indicated $\lambda(G) = \|(2,1,1);\ (1,2,1);\ 3\cdot(3,1,0)\|$. In a slightly changed form $\lambda(G)$ is called a distance degree sequence of a graph that for the graph in Fig.2 has the following form $DDS(G) = (\ (2,1,1),\ (1,2,1), (3,1,0)^3)$ [3].

Let us show some simple properties of the layer matrix $\lambda(G)$ [2,4].

1. Let $\lambda_G(v)$ be the matrix $\lambda(G)$ line corresponding to the partition $\hat{G}(v)$. The line length is then equal to $e(v)$ that is the matrix line lengths form the eccentric sequence of graph G.

2. Let $\lambda_G(v)$ be the the i-th line of $\lambda(G)$. Then $\sum_{j=1}^{e(v)} \lambda_{ij} = p-1$, $\lambda_{ij} > 0$, $1 \leq j \leq e(v)$.

3. At least two first lines of the canonic layer matrix have a length of a graph diameter. The last line length is equal to the radius of a graph.

4. First column $\lambda(G)$ is the graph degree sequence, $\sum_{i=1}^{p} \lambda_{i1} = 2q$.

5. A layer matrix is connected with a distance matrix in the following way - the matrix element λ_{ij} is equal to the number of elements being equal to j in the line of the distance matrix for the vertex i.

6. From an equality of matrices of the second order does not follow an equality of the layer matrices of the first order. In fact, $\lambda^2(K_4 - v) = \lambda^2(K_4)$, $\lambda(K_4 - v) \neq \lambda(K_4)$.

7. From the equality of the layer matrices $\lambda(G) = \lambda(H)$ does not follow that $G \simeq H$. Figs. 3a,b show the examples of nonisomorphic trees [2,5], and Fig. 3,c - the examples of nonisomorphic graphs (with an identity automorphism group) with the

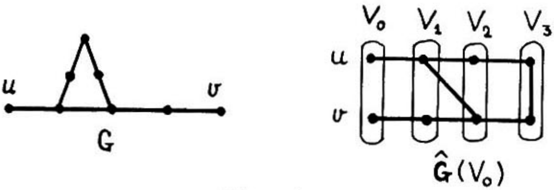
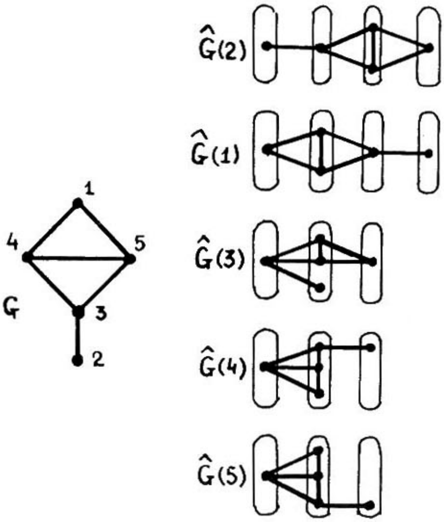


Fig. 1



$$\lambda(G) = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \left\| \begin{array}{ccc} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 3 & 1 & 0 \\ 3 & 1 & 0 \\ 3 & 1 & 0 \end{array} \right\|$$

$$\lambda_X(G) = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \left\| \begin{array}{ccc} 2 & 2 & 1 \\ 1 & 2 & 2 \\ 3 & 2 & 0 \\ 3 & 1 & 0 \\ 3 & 1 & 0 \end{array} \right\|$$

Fig. 2

same layer matrices.

8. An equality of the complete layer matrices $\lambda_G(V,X)=\lambda_H(V,X)$ does not provide that $G \simeq H$. Fig. 4 shows nonisomorphic graphs with the same complete layer matrices. The same property is posessed, for example, by Moore's graphs having the same order and degree of vertices.

9. From the pair coincidence of the vertex layer matrices of the same order for the whole family of matrices $\lambda^n(G)$, $n=1,2...$ an isomorphism of graphs does not come. Fig.5 shows nonisomorphic graphs G and H for which $\lambda^i(G)=\lambda^i(H)$ is valid for $1 \leq i \leq 4$. In fact, $\lambda^1(G)=\lambda^1(H)= \| 3\cdot(2,2);\ 2\cdot(3,1) \|$, $\lambda^2(G)=\lambda^2(H)= \| 3\cdot(2,1);\ 7\cdot(3) \|$; $\lambda^3(G)=\lambda^3(H)= \| 10\cdot(2) \|$, $\lambda^4(G)=\lambda^4(H)= = \| 5\cdot(1) \|$.

10. There are not only single examples but also classes of graphs that are not defined unambiguously by their layer matrices. Such a class of graphs, for example, forms regular graphs as G and H of a degree z and diameter two for which the following condition is valid $\lambda(G)=\lambda(H)=\| p\cdot(z, p-z-1) \|$.

11. There are nonisomorphic graphs G and H for which the following condition is satisfied $\lambda^2_G(V,X)=\lambda^2_H(V,X)$.

12. There are nonisomorphic graphs G and H for which $\lambda(G-v_i)=\lambda(H-u_i)$ is valid for all $i=1,2,...,p$ and $\lambda(G)=\lambda(H)$ where graph $G-v$ is obtained from graph G by the deleting vertex v and all the edges incident to v.

13. It is interesting to define nonisomorphic graphs G and H such as the condition $\lambda(G-v_i)=\lambda(H-u_i)$ is valid for all $i=1,2...,p$ but $\lambda(G)\neq\lambda(H)$.

14. In reference [5] the conditions are considered under which the integer number matrix λ given will be the layer matrix

of some tree and an algorithm was suggested for the construction of trees having the same layer matrix as λ . Note, that in addition to the simplest relations between the layer matrix elements, the graphic condition should be satisfied both for the degree sequence of a graph (first column of layer matrix) and for its eccentricity sequence which is formed by the lengths of the layer matrix lines.

2. ISOMETRICITY OF GRAPHS

The isometric graphs are defined and some properties of graphs are considered in Ref. [6]. The relation of isometricity in the class of equivalence on the metric properties of graphs is analogous to the relation of isomorphism on the set of graphs. The necessary and sufficient conditions are established in Ref.[7] for the isometricity which give a simple with respect to calculation and constructive criterion for establishing an isometricity of graphs.

DEFINITION 3 [7]. ℓ -spectrum of graph G is called a matrix $\ell(G)$ which consists of all the mutually different pairs of lines of the layer matrix $\lambda(G)$.

The matrix $\ell(G)$ has a canonic form similar to that of matrix $\lambda(G)$. The number of lines in $\ell(G)$ is denoted as $|\ell(G)|$. Apparently, the graph, for which the condition $\ell(G)=\lambda(G)$ is valid, has the only identity automorphism. If $\ell(G)$ consists of one line, $|\ell(G)| = 1$, then all the vertices of graph are metrically equivalent. In Ref.[3] the graphs with $\ell(G) = \lambda(G)$ and $|\ell(G)|=1$ are called the graphs with injective and regular distance degree sequences. Let graphs G and H have the same order.

DEFINITION 4 [6]. Graph H is isometric from graph G, $G \rightsquigarrow H$, if for every vertex $v \in V(G)$ one can define a one-to-one correspondence of $V(G)$ to $V(H)$ $\varphi_v : V(G) \to V(H)$ such that for any $u \in V(G)$ $d_G(v,u) = d_H(\varphi_v(v), \varphi_v(u))$.

Graphs G and H are called isometric, if $G \rightsquigarrow H$ and $H \rightsquigarrow G$ which is denoted as $G \leftrightarrow H$. The isometricity and ℓ-spectra are related as follows.

THEOREM 1 [7]. $G \leftrightarrow H \Leftrightarrow \ell(G) = \ell(H)$.

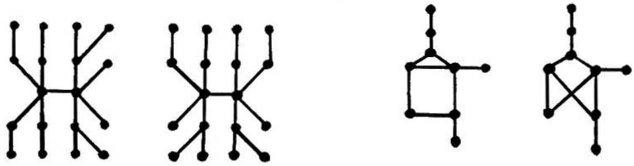
Thus, ℓ-spectra of graphs characterize completely the isometric graphs. Note, that isometric graphs can have different layer matrices. Fig. 6 shows nonisomorphic isometric graphs for which: $\ell(G) = \ell(H) = \|(3,1);(2,2)\|$ and $\lambda(G) = \|2,3,4,5\,(3,1);1\,(2,2)\|$, $\lambda(H) = \|2,3\,(3,1);1,4,5\,(2,2)\|$.

Correspondences φ_v produce the permutations on the vertex set of graphs G and H conserving the property of isometricity. Such permutations will be called the isometricity permutations of graphs G and H. A set of all the permutations denote as $I_\ell(G,H)$. In order to define all the isometricity permutations it is sufficient to consider all the single vertex relative partitions. Let $\hat{G}(v)$, $\hat{H}(u)$ be relative partitions and lines $\lambda_G(v)$ and $\lambda_H(u)$ in the layer matrices be the same, then for the layers $V_i(v)$ and $V_i(u)$, $0 \le i \le e(v)$ relation $\varphi_v(V_i(v)) = V_i(u)$ is satisfied where for $U \subseteq V(G)$ the value of $\varphi_v(U)$ is defined as $\varphi_v(U) = \bigcup_{w \in U} \varphi_v(w)$.

The total number of the isometricity permutations for graphs G and H is given by the formula

$$|I_\ell(G,H)| = \sum_{i=1}^{|\ell(G)|} a_i(G)\,a_i(H) \prod_{j=1}^{K_i} \ell_{ij}! \quad ,$$

a)



b) c)

Fig. 3

Fig. 4

Fig. 5

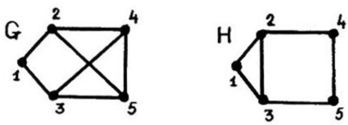
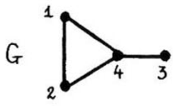


Fig. 6

Fig. 7



$$\lambda(G) = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \left\| \begin{array}{cc} 2 & 1 \\ 2 & 1 \\ 1 & 2 \\ 3 & 0 \end{array} \right\| \qquad \tau(G) = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \left\| \begin{array}{ccc} 2 & 3 & 1 \\ 2 & 3 & 1 \\ 1 & 2 & 2 \\ 3 & 2 & 0 \end{array} \right\|$$

Fig. 8

where $a_i(G)$, $a_i(H)$ is the value of multiplicity for i -th line $\ell(G)$ in the layer matrices $\lambda(G)$ and $\lambda(H)$ respectively, ℓ_{ij} - the value of j -th element of i -th line $\ell(G)$, K_i is a length of i -th line. For graphs given in Fig.6 $|I_\ell(G,H)|=60$. It is evident that an arbitrary graph is isometric to itself. In this case, the isometricity permutation will be called the auto-metricity permutation. The number of such permutations is determined by the spectrum $\ell(G)$. The total number of autometricity permutations is

$$|A_\ell(G)| = \frac{1}{2}\sum_{i=1}^{|\ell(G)|} a_i(a_i+1)\prod_{j=1}^{K_i} \ell_{ij}! \quad .$$

The value of $|A_\ell(G)|$ takes its minimum when all the layer matrix lines $\lambda(G)$ are different i.e. at $\ell(G)=\lambda(G)$. In this case, $|A_\ell(G)| = \sum_{i=1}^{|\ell(G)|}\prod_{j=1}^{K_i}\ell_{ij}!$. $|A_\ell(G)|$ takes its maximum value on the graphs where $|\ell(G)|=1$. In this case $|A_\ell(G)|$ = $= \frac{1}{2}p(p+1)\prod_{j=1}^{d(G)}\ell_{ij}!$, where $d(G)$ is a diameter of graph G.

3. LAYER MATRIX AND METRIC CHARACTERISTICS OF GRAPHS

Many properties of graphs are determined by the shortest distances between its vertices. Based on a distance concept $d(u,v)$ $u,v \in V(G)$ are the graph metric characteristics as the functions of the graph parameters and the distances between its vertices. Among the metric characteristics one can distinguish two classes as the eccentric and distance characteristics [4].

3.1 ECCENTRIC CHARACTERISTICS

This class of graph characteristics is based on the concept of the vertex eccentricity. Some eccentric characteristics are given in Table 1. Depending on the values of graph characteristics

Table 1

No	Designation	Name	Expressions for calculation
1	$e(v)$	Vertex eccentricity [8]	$e(v)=\max\limits_{u\in V(G)} d(u,v)$
2	$r(G)$	Radius of a graph [8]	$r(G)=\min\limits_{v\in V(G)} e(v)$
3	$d(G)$	Graph diameter [8]	$d(G)=\max\limits_{v\in V(G)} e(v)$
4	$e(G)$	Eccentricity of graph [4]	$e(G)=\sum\limits_{v\in V(G)} e(v)$
5	$e_{av}(G)$	Average vertex eccentricity in graph [4]	$e_{av}(G)=\frac{1}{p}\, e(G)$
6	$\Delta e(v)$ $\bar{\Delta} e(v)$	Eccentric of vertex [4]	$\Delta e(v)=\lvert e(v)-e_{av}(G)\rvert$ $\bar{\Delta} e(v)= e(v)-e_{av}(G)$
7	ΔG	Eccentric of graph [4]	$\Delta G=\frac{1}{p}\sum\limits_{v\in V(G)} \Delta e(v)$

Table 2

No	Designation	Name	Expressions for calculation
1	2	3	4
1	$D(v)$	Distance of a vertex [9] (vertex centrality [10])	$D(v) = \sum_{u \in V(G)} d(v,u)$
2	$D(G)$	Distance of a graph [9] (graph integration [10])	$D(G) = \frac{1}{2} \sum_{v \in V(G)} D(v)$
3	$D^*(v)$	Minimal distance of a graph [4] (unipolarity [10])	$D^*(G) = \min_{v \in V(G)} D(v)$
4	$\Delta D^*(v)$	Distance vertex deviation from its minimum [4]	$\Delta D^*(v) = D(v) - D^*(G)$
5	$var(G)$	Variation of a graph [4]	$var(G) = \max_{v \in V(G)} \Delta D^*(v)$
6	ΔG^*	Distance graph deviation [4] (centralization [10])	$\Delta G^* = \sum_{v \in V(G)} \Delta D^*(v) = 2D(G) - pD^*(G)$
7	$D_{av}(G)$	Average distance of graph vertices [4]	$D_{av}(G) = \frac{2D(G)}{p}$
8	$\Delta D(v)$ $\bar{\Delta} D(v)$	Distance vertex deviation from average [4]	$\Delta D(v) = \lvert D(v) - D_{av}(G) \rvert$ $\bar{\Delta} D(v) = D(v) - D_{av}(G)$

Table 2 (continued)

1	2	3	4
9	$\Delta D(G)$	Mean distance deviation of a graph [4]	$\Delta D(G) = \frac{1}{p} \sum_{v \in V(G)} \Delta D(v)$
10	$m_1(v)$	Mean deviation of a graph vertex [11]	$m_1(v) = \frac{1}{p} D(v)$
11	$m_2(v)$	Mean square deviation of a graph vertex [11]	$m_2(v) = \frac{1}{p} \sum_{u \in V(G)} [d(u,v)]^2$
12	$m_2^*(G)$	Graph dispersion [11]	$m_2(G) = \min_{v \in V(G)} m_2(v)$
13	$D^{-1}(v)$	Converse distance of a vertex [4]	$D^{-1}(v) = \frac{1}{D(v)}$
14	$D^{-1}(G)$	Converse distance of a graph [4]	$D^{-1}(G) = \frac{1}{D(G)}$
15	$D^{*-1}(G)$	Converse minimal distance [4]	$D^{*-1}(G) = \max_{v \in V(G)} D^{-1}(v)$
16	$L(G)$	Converse centralization [4]	$L(G) = \sum_{v \in V(G)} (D^{*-1}(G) - D^{-1}(v)) = p D^{*-1}(G) - 2 D^{-1}(G)$
17	$\mu(G)$	Compactness of a graph (mean distance [12]	$\mu(G) = \frac{1}{\binom{p}{2}} \sum_{u,v \in V(G)} d(u,v) = \frac{4}{p(p-1)} \cdot D(G)$

one can separate in the graph some certain vertex sets and respectively induced subgraphs. Such nonnumerical characteristics will be called the graph constructions. The well known graph constructions are the following - center of a graph is a set vertices $v \in V(G)$ for which the relation $e(v) = r(G)$ is valid, graph periphery is a set of $v \in V(G)$ for which $e(v) = d(G)$ is valid and others.

3.2 DISTANCE CHARACTERISTICS

This class of characteristics is based on the concept of the graph vertex distance. Some distance characteristics are given in Table 2.The constructions of a graph include such as a median of graph that assumes a set of $v \in V(G)$ for which the relation $D(v) = D^{*}(G)$ is valid, the graph center of gravity assuming a set of $v \in V(G)$ with $m_2(v) = m_2^{*}(G)$ satisfied and others.

Metric characteristics of graphs have been studied in many papers with major attention paid to obtaining the upper and lower bounds for the graph distance $D(G)$, graph compactness $\mu(G)$ etc. A bibliography of 37 papers on the subjects is given in Ref.[13].

3.3 LAYER MATRIX AND METRIC CHARACTERISTICS CALCULATIONS

The use of the layer matrix of graph $\lambda(G)$ enables one to utilize a unified method for calculation of metric characteristics. A function calculable on matrix $\lambda(G)$ let us call the λ-calculable. From the matrix properties if comes immediately that the line length is equal to the eccentricity of corresponding vertex. The first line length is equal to the diameter value and the latter-to radius of the graph. Thus, the eccentricity characteristics are λ-calculable. Since the distance characteristics are calculated through the vertex distances, their λ-calculability follows from the λ-calculability of $D(v)$, $v \in V(G)$.

Let vertex v in matrix $\lambda(G)$ correspond to the i-th line, then,

$$D(v) = \sum_{j=1}^{e(v)} j \cdot \lambda_{ij} \quad .$$

This formula can be used both for direct calculation and also for obtaining analytic expressions for metric characteristics of graphs. Let us give some examples. Let C_p be a simple cycle of the order p, then if p is even, $\lambda(C_p) = \| p \cdot (\underbrace{2, 2, \ldots, 2}_{(p-2)/2+1}, 1) \|$ and $D(C_p) = \frac{1}{8} p^3$, if p is odd, $\lambda(C_p) = \| p \cdot \underbrace{(2, 2, \ldots, 2)}_{(p-1)/2} \|$ and $D(C_p) = \frac{1}{8}(p^2-1)p$. If K_p is a complete graph of the order p, then $\lambda(K_p) = \| p \cdot (p-1) \|$ and $D(K_p) = \frac{1}{2} p(p-1)$

For the complete bipartite graph $K_{m,n}$, $\lambda(K_{m,n}) = \| m \cdot (n, m-1);$ $n \cdot (m, n-1) \|$ whence $D(K_{m,n}) = n \cdot m + n(n-1) + m(m-1)$.

The characteristics can be calculated by the spectrum $\ell(G)$. Such characteristics called as ℓ-spectral are used for studies of the symmetry properties of graphs determined by the isometricity relation by the comparison of characteristics obtained with $\ell(G)$ and $\lambda(G)$. In Ref. [14] the graph complexity function is considered for

$$\xi(G) = \frac{pq}{p+q} \sum_{\substack{i,j \\ i<j}} \gamma(i,j) \quad ,$$

where $\gamma(i,j)$ is the number of various paths from the vertex i to j. It is indicated that $\xi(G)$ has the following properties: monotonically increases both with number of vertices and edges of a graph; displays the graph connectivity degree; corresponds to the intuitional concept of complexity by matching large numbers to graphs which "look" as complex and vice versa. Let us show that $\xi(G)$ is not a λ-calculable. In fact, for the graphs given in Fig. 7 $\lambda(G) = \lambda(H) = \| 2\cdot(2,2,1);\ 3\cdot(3,2) \|$, but $\xi(G) \neq \xi(H)$ since $\xi(G) = 260.2$ and $\xi(H) = 274.3$.

4. PATH LAYER MATRIX AND PATH CHARACTERISTICS OF GRAPHS

One can obtain some interesting properties of graphs by studying sets of paths of graphs. A path connecting vertices $v_1, v_k \in V(G)$ is called a sequence of the pair mutually different vertices $v_1, v_2, \ldots, v_{k-1}, v_k$, $(v_i, v_{i+1}) \in X(G)$, $i = 1,2,\ldots,k-1$. The length of the longest path connecting vertices $u, v \in V(G)$ is called an elongation $el(u,v)$ between the vertices [11]. The maximum elongation value for the graph vertices is called the graph elongation diameter.

<u>DEFINITION 5</u> [15]. The sum of lengths of all the possible paths connecting vertices u and v is called a path distance $p(u,v)$ between vertices $u, v \in V(G)$.

Analogous to the layer matrix $\lambda(G)$ let us define the path layer matrix for the graph $\tau(G)$.

<u>DEFINITION 6</u> [16]. The matrix $\tau(G) = \|\tau_{ij}\|$, $i = 1,2,\ldots,p$, $j = 1,2,\ldots, d_\tau(G)$, where τ_{ij} is the number of various paths of a length j coming from i-th vertex, $d_\tau(G)$ is an elongation diameter G is called the path layer matrix of graph G.

The length of a line corresponding to i-th vertex let us call such a maximum value of j that $\tau_{ij} \neq 0$. The canonic form of a matrix $\tau(G)$ and its representation in linear form is defined similarly to that of the layer matrix $\lambda(G)$. Fig. 8 shows the graph and its matrices $\lambda(G)$ and $\tau(G)$. If G is a tree, then $\tau(G) = \lambda(G)$ since any two vertices of a tree are connected by the unique path. Matrix $\tau(G)$ contains more complete information on graph than $\lambda(G)$. For graphs given in Fig. 5 the layer matrices of any order are the same, but

$\tau(G) = \| (2,4,4,4);\ 2\cdot(2,3,5,3);\ 2\cdot(3,4,2,0) \|$,

$\tau(H) = \| 3\cdot(2,4,4,4);\ 2\cdot(3,3,4,0) \|$.

In Ref.[3] matrix $\tau(G)$ is considered as the path degree sequence of the graph PDS (G). For some graphs the layer matrix can be given in explicit form. For example, for the complete graph K_p the path layer matrix has the form $\tau(K_p) = \| p\cdot(p-1, (p-1)(p-2), (p-1)(p-2)(p-3), \ldots, (p-1)!) \|$, for a cycle of the order p $\tau(C_p) = \| p\cdot(\underbrace{2,2,\ldots,2}_{p-1}) \|$ or the complete bipartite graph $K_{m,n}$ $\tau(K_{m,n}) = \| m\cdot(a_1, a_2, \ldots, a_k);\ n\cdot(b_1, b_2, \ldots, b_t) \|$, where

$$b_\tau = \begin{cases} \dfrac{m!}{(m-\frac{\tau+1}{2})!}\cdot\dfrac{(n-1)!}{(n-\frac{\tau+1}{2})!}, & \tau \quad \text{odd} \\[2ex] \dfrac{m!}{(m-\frac{\tau}{2})!}\cdot\dfrac{(n-1)!}{(n-\frac{\tau+2}{2})!}, & \tau \quad \text{even} \end{cases}$$

The values for a_τ are obtained from the expression for b_τ by mutual exchange of values m and n. If $m<n$ then $k=2m-1$, $t=2m$ and with $n<m$ $k=2n$, $t=2n-1$.

Let us consider the uniquness of presentation of graphs with the path layer matrices. In Ref. [16] is shown that an equality of the path layer matrices for the graphs of the order not in access of 11 is the condition sufficient for their isomorphism. In Ref.[2] an example has been given of nonisomorphic trees of the order 23 having the same path layer matrices (Fig. 3a) and in Ref.[5] the trees are given which apparently have the smallest order (Fig. 3b). Ref. [17] presents a procedure for constructing such trees. Ref. [15] indicates that nonisomorphic graphs with the same layer matrices including the given graph G as a subgraph can be obtained with the method examplidied in Fig. 9. Ref. [18] studies possible values of girth and cyclic rank for similar graphs. The length of the smallest cycle is called a graph girth. The value of $\beta = q - p + 1$ is called a cyclic rank of the connected graph. The value β is also interpreted as the number of independent cycles in a graph. In Ref. [18] the following assumption is formulated:

The lowest order for which there is a pair of nonisomorphic connected graphs having similar path layer matrices is equal to

(1) $16 + g$ if the graph girth is g

(2) $16 + \left\lceil \frac{3+\sqrt{1+8\beta}}{2} \right\rceil$ if graphs have β independent cycles, $\lceil S \rceil$ denotes the minimal integer larger or equal to S .

Fig. 10 shows pairs of nonisomorphic graphs satisfying the conditions of the assumption. To the assumption given above let us give a negative answer. Actually, graphs shown in Fig. 11 having the order p = 18, girth g = 4 and cyclic rank β = 2 are the counter expamples for the assumption. The path layer matrix for these graphs has the form τ = ‖ 15,16 (1,3,6,11,14,7,6,2); 1 (1,2,7,12,12,10,6,2); 2 (1,2,5,12,16,10,6,2); 17,18(1,2,4,8, 10,8,8,2); 3,4(1,1,4,9,10,8,8,2); 11 (4,6,11,14,7,6,2); 5 (3,7,12,12,10,6,2); 6 (3,5,12,16,10,6,2); 12(3,4,8,10,8,8,2); 13 (2,6,13,14,13,6,2); 8,7 (2,4,9,10,8,8,2); 14(1,4,10,10,8,8,2): 9,10 (5,10,10,8,8,2)‖ .

Graphs given in Fig. 12 are also the counter examples for the assumption. The order of graphs is p = 18, girth g = 4 and cyclic rank β = 4. The path layer matrix has now the form τ =

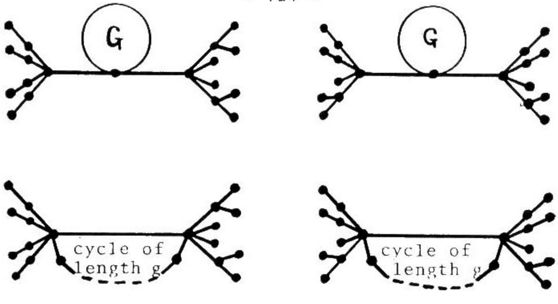


Fig. 9

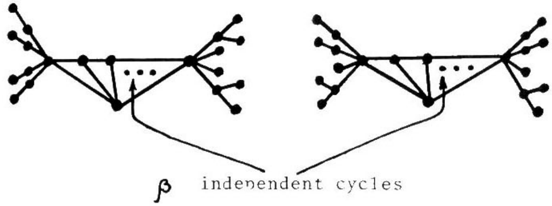


Fig. 10

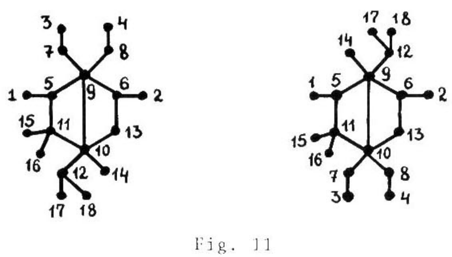


Fig. 11

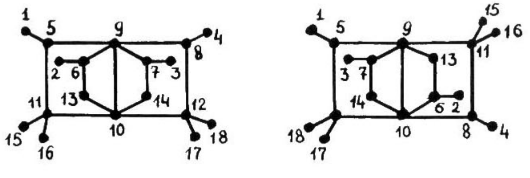


Fig. 12

=‖15,16,17,18(1,3,6,13,22,21,24,14,6); 1,4(1,2,7,14,20,24,24,18,4); 2,3(1,2,5,14,24,24,24,18,8); 11,12(4,6,13,22,21,24,14,6); 5,8(3,7,14,20,24,24,18,4); 6,7(3,5,14,24,24,24,18,8); 13,14(2,6, 15,22,27,24,22,6); 9,10(5,12,16,16,24,12)‖.

These examples of graphs are obtained from the trees in Fig. 3b. And again as previously we do not know anything of graphs with the same path layer matrices which are not obtained with any method from the trees with the same layer matrices.

5. PATH CHARACTERISTICS OF GRAPHS

For graphs one can define a class of characteristics based on the consideration of the graph path sets. Such characteristics will be called the path characteristics. The path characteristics are divided into two classes: the elongation characteristics and τ -distance characteristics.

The elongation characteristics are based on the concept of elongation between two graph vertices $el(u,v)$ $u,v \in V(G)$. Such graph characteristics as the radius and diameter of elongation are known [11]. The value $e_\tau(v) = \max\limits_{u \in V(G)} el(u,v)$ we shall call the path eccentricity of vertex $v \in V(G)$. Since $d(u,v) \leq$ $\leq el(u,v) \leq p-1$ it is evident that $e(v) \leq e_\tau(v) \leq p-1$. Using $e_\tau(v)$ in place of $e(v)$ one can define the set of elongation characteristics corresponding to the eccentricity characteristics.

The calss of the τ -distance characteristics is based on the concept of the path distance in a graph. Similar to that as the distance characteristics are constructed with the use of $D(v)$, $v \in V(G)$, τ -distance characteristics are constructed on the base of the τ -distance vertices $D_\tau(v)=\sum_{u\in V(G)} \rho(u,v)$, $v\in V(G)$ .The use of the path characteristics enables one to get the more complete information on the graph structure compared to the metric characteristics.

The path characteristics are τ -calculable. From the properties of $\tau(G)$ immediately follows that the line length in $\tau(G)$ is equal to the elongation number of the corresponding vertex. The length of no less than two first lines is equal to the graph elongation diameter, the latter line length is equal to the graph elongation radius. Thus all the characterisitcs are τ -calculable. The vertex distances are also calculable. If in $\tau(G)$ to the vertex $v\in V(G)$ corresponds i -th line, then $D_\tau(v)=\sum_{j=1}^{e_\tau(v)} j\cdot\tau_{ij}$.

Knowing the evident form of $\tau(G)$ one can obtain formulas for values of τ -characteristics. For example, since $D_\tau(G)$ = $\frac{1}{2}\sum_{v\in V(G)} D_\tau(v)$, then by the given above values of $\tau(C_p)$,$\tau(K_p)$ we obtain $D_\tau(C_p)=\frac{1}{2}p\sum_{j=1}^{p-1} 2\cdot j = \frac{1}{2}p^2(p-1)$, $D_\tau(K_p)$ =

$$\frac{1}{2}p[(p-1)+2(p-1)(p-2)+\ldots+(p-1)(p-1)!] = \frac{1}{2}p(p-1)!\sum_{\tau=1}^{p-1}\frac{\tau}{(p-\tau-1)!} .$$

A graph complexity function $\xi(G)$ is the τ -calculable. Actually, through the components τ_{ij} of matrix $\tau(G)$ the function $\xi(G)$ is expressed in the following form:

$$\xi(G)=\frac{pq}{2(p+q)}\sum_{i=1}^{p}\sum_{j=1}^{e_\tau(i)}\tau_{ij}(G) .$$

By this formula we obtain the values of $\xi(G)$ for graphs K_p , C_p and for a tree T_p of the order p . One has

$$\xi(C_p)=\frac{p^2}{2p}\cdot\frac{1}{2}\sum_{i=1}^{p}\sum_{j=1}^{p-1}\tau_{ij}(C_p)=\frac{p}{4}\sum_{i=1}^{p}\sum_{j=1}^{p-1}2=\frac{1}{2}p^2(p-1)\ ,$$

$$\xi(T_p)=\frac{p(p-1)}{2\cdot p-1}\cdot\frac{1}{2}\sum_{i=1}^{p}\sum_{j=1}^{e(i)}\tau_{ij}(T_p)=\frac{p(p-1)}{2(2p-1)}\sum_{i=1}^{p}(p-1)=\frac{p^2(p-1)^2}{2(2p-1)}\ ,$$

$$\xi(K_p)=\frac{p(p-1)}{2(p+1)}\sum_{i=1}^{p}\sum_{j=1}^{p-1}\tau_{ij}(K_p)=\frac{p(p-1)}{2(p+1)}p[(p-1)+(p-1)(p-2)+\ldots+$$

$$(p-1)!]=\frac{p^2(p-1)}{2(p+1)}\sum_{\tau=0}^{p-2}\frac{(p-1)!}{(p-\tau-1)!}=\frac{p^2(p-1)}{2(p+1)}\cdot(p-1)!\sum_{\tau=0}^{p-2}\frac{1}{(p-\tau-2)!}\ .$$

The values obtained coincide with the values $\xi(G)$ for the indicated graphs given in Ref.[14]. Knowing the evident form of $\xi(G)$ one can see how the values are connected with the path and metric characteristics. For example, for C_p $\xi(C_p)=D_\tau(C_p)$ and

$$\xi(C_p)=\begin{cases} D(C_p)\cdot\dfrac{4(p-1)}{p}\ , & p \text{ even} \\[2ex] D(C_p)\cdot\dfrac{4p}{p+1}\ , & p \text{ odd}\end{cases}$$

Note that if $\tau(G)=\tau(H)$, then $\xi(G)=\xi(H)$, but inversely it does not hold. In Fig. 13 one can find that for graphs G and H $\xi(G)=\xi(H)$, but $\tau(G)\neq\tau(H)$. For these graphs $\xi(G)=\xi(H)=$ $=26676$ and the first lines of matrices $\tau(G)$ and $\tau(H)$ have the form $\tau_1(G)=(4,12,34,70,142,254,300,156)$, $\tau_1(H)=(4,12,32,74,152,258,294,164)$.

6. ISOTOPICITY OF GRAPHS

Let us consider the question of the existence of a graph correspondence which conserves the path distance between the graph vertices.

The path distribution for the vertices $u,v \in V(G)$ of a graph G of the order p we shall call a sequence $\alpha(u,v) = (\alpha_1,\alpha_2,\dots,\alpha_{p-1})$, where α_i is the number of paths of a length i connecting vertices u and v. The path distance between u and v can be represented in the form $\rho(u,v) = \sum_{i=1}^{p-1} i\cdot\alpha_i$.

DEFINITION 7. [15] The graph H is isotopic from the graph G, $G \approx> H$, if for every vertex $v \in V(G)$ there is a one-to-one correspondence $V(G)$ upon $V(H)$ $\varphi_v : V(G) \to V(H)$ such that for any $u \in V(G)$ the equality $\alpha_G(v,u) = \alpha_H(\varphi_v(v),\varphi_v(u))$ is satisfied.

The graphs G and H are isotopic, $G \Leftrightarrow H$, if $G \approx> H$ and $H \approx> G$. The conservation of the path distribution in the isotopic graphs causes the conservation both of the path distance between the vertices and other distances based on the path distribution of vertices.

Let us associate the vertex $v_i \in V(G)$ with the square matrix of the order $p-1$

$$R(v_i) = \left\| \begin{matrix} \alpha(v_i,v_1) \\ \cdots \\ \alpha(v_i,v_{i-1}) \\ \alpha(v_i,v_{i+1}) \\ \cdots \\ \alpha(v_i,v_p) \end{matrix} \right\|$$

The matrix $R(v_i)$ will be given in the same canonic form similar to that as for the path layer matrix $\tau(G)$.

DEFINITION [15]. The set of paired different matrices from the set $\{R(v)\}$, $v \in V(G)$ is called the S-spectrum of the graph G.

If for any matrix from $S(G)$ there is the same matrix in

$S(H)$ and vice versa, we shall say that the S-spectra of graphs coinside $S(G)=S(H)$.

THEOREM 2 [15]. $G \Leftrightarrow H \Leftrightarrow S(G)=S(H)$.

For the trees the isotopicity concept is equivalent to isometricity.

COROLLARY. If G and H are the trees, then $G \Leftrightarrow H \Leftrightarrow G \leftrightarrow H$.
In the general case this statement is not valid. The graphs given in Fig. 5 have the same layer matrices of all orders but they are not isotopic. The coincidence of the sets of the paired different lines in the path layer matrices is only the necessary condition for the isotopicity as $\tau_{ij}=\sum_{\substack{k=1\\k\neq i}}^{p-1} d_j(v_i,v_k)$,

where $d_j(u,v)$ is the j-th component $d(u,v)$, i.e. τ_{ij} is equal to the sum of elements in the j-th column of the matrix $R(i)$.

The graphs given in Fig.9 are isotopic. Correspondences φ_v induce the isotopicity permutations on the graph vertex set. The total number of the isotopicity permutations $I_S(G,H)$ for graphs G and H is given by the formula

$$I_S(G,H)=\sum_{i=1}^{|S(G)|} m_i(G)\, m_i(H) \prod_{j=1}^{n_i} s_{ij}!\ ,$$

where $|S(G)|$ is the number of matrices in $S(G)$, $m_i(G)$ and $m_i(H)$ are the multiplicities of the i-th matrix $S(G)$ in $\{R(v)\}, v\in V(G)$ and $\{R(u)\}, u\in V(H)$, s_{ij} is the number of lines in a j-th block of similar lines in the i-th matrix $S(G)$, n_i is the number of such blocks in the matrix.

7. RELATIVE METRIC CHARACTERISTICS

In many problems of the structural information processing the problem arises of the metric characterization not only for the whole graph but also for its parts as subgraphs, partial subgraphs, sets of vertices, etc. Let us use the metric characteristics for describing the subgraph position in the graph.

Let $V_0 \subseteq V(G)$, $H \subseteq G$, $D_{V_0}(H) = \sum\limits_{\substack{v \in V(H) \\ u \in V_0}} d(u,v)$,

$e_{V_0}(H) = \sum\limits_{v \in V(H)} \max\limits_{u \in V_0} d(u,v)$.

DEFINITION 8. The subgraph (normalized) distance $H \subseteq G$ in the graph G with respect to the set $V_0 \subseteq V(G)$ is called the function

$$D(H,V_0) = \frac{1}{D(G)} \cdot D_{V_0}(H) .$$

Similarly defined is the eccentricity H in G with respect to $V_0 \subseteq V(G)$ $e(H,V_0) = \frac{1}{e(G)} \cdot e_{V_0}(H)$. Such characteristics which we shall call the relative ones enable us to describe the subgraph position with respect to the distinguished vertex set of a graph taking into account the characteristics of the whole graph. The relative posiiton of the subgraph can be described with the help of any other characteristics. Let $V_0 = V(G)$ then the value $D(H,V_0)$ characterizes the position of the subgraph H in G . Let us give the simple values for $e(v)/e(G)$ and $D(v)/D(G)$, $v \in V(G)$. One should note that the values $e(v)$, $e(G)$ and $D(v)$, $D(G)$, $v \in V(G)$ are mutually dependent.

THEOREM 3. Let G be a graph of the order p and $v \in V(G)$ then

$$\frac{1}{2p} \leqslant \frac{e(v)}{e(G)} \leqslant \frac{2}{p} .$$

PROOF. For any $v \in V(G)$ an inequality $r(G) \leq e(v) \leq d(G)$ or $p r(G) \leq e(G) \leq p d(G)$ is valid where $r(G)$, $d(G)$ are the radius and diameter of G respectively. Let us divide the latter inequality by $e(v)$: $p\frac{r(G)}{e(v)} \leq \frac{e(G)}{e(v)} \leq p\frac{d(G)}{e(v)}$ (*)
Substituting $e(v)$ in the left part of (*) by $d(G)$ in the right part by $r(G)$ and taking into account that $d(G) \leq 2r(G)$ we get $\frac{p}{2} \leq \frac{e(G)}{e(v)} \leq 2p$ or $\frac{1}{2p} \leq \frac{e(v)}{e(G)} \leq \frac{2}{p}$. The theorem is proved.

Let us give the examples of graphs where the value of $e(v)/e(G)$ is close to the upper and lower bounds of the Theorem 3. Let $v \in V(K_p - x)$ where K_p is a complete graph of the order p, $x \in X(K_p)$. Let us choose v such as that $\deg v = p-2$, then $\frac{e(v)}{e(G)} = \frac{2}{p+2}$.

Let H be a regular graph of the order p of the degree $p-2$. Such a graph can be obtained, for example, from K_p of even order by deleting $p/2$ edges. Let us form the graph $L = H + x$, where x is a new edge, $x \notin X(H)$. For the vertex $v \in V(L)$ with $\deg v = p-1$ we get $\frac{e(v)}{e(G)} = \frac{1}{2p-2}$.

Let Q be a set of all graphs of the order p with a diameter d. Let us denote $D_{min} = \min_{G \in Q} \min_{v \in V(G)} D(v)$, $D_{max} = \max_{G \in Q} \max_{v \in V(G)} D(v)$.

LEMMA 1.

$$D_{max} = pd - \tfrac{1}{2}d(d+1),$$
$$D_{min} = \tfrac{1}{2}d\left(\tfrac{d}{2} - 1\right) + p - c,$$

where $c = 1$, if d is even and $c = 3/4$ if d is odd.

PROOF. In the graph of a diameter d there is the shortest path of a length d between the diametric vertices.

Among the vertices of a simple path the central vertex v

Fig. 13

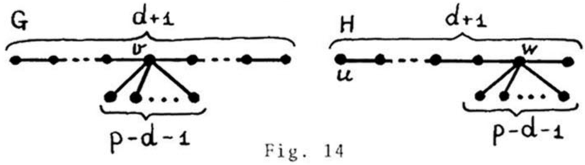


Fig. 14

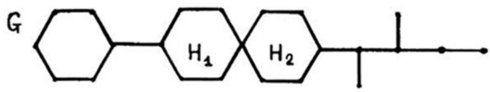


Fig. 15

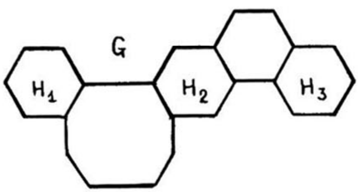


Fig. 16

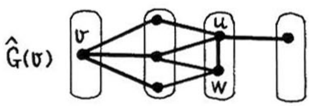
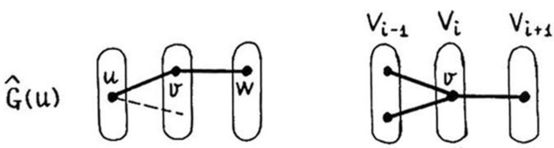


Fig. 17



a) b)

Fig. 18

has a minimal distance. Let the remaining vertices $p-d-1$ which are not included into this path of a length d be located at a distance one from the vertex v. As follows from the construction $D(v)=D_{min}$, $D(v)=\frac{1}{2}(\frac{d}{2}+1)\frac{d}{2}+\frac{1}{2}(\frac{d}{2}+1)\frac{d}{2}+$ $+(p-d-1)=\frac{d}{2}(\frac{d}{2}-1)+p-1$,

if d is even and $D(v)=\frac{1}{2}(\frac{d-1}{2}+1)\frac{d-1}{2}+\frac{1}{2}(\frac{d+1}{2}+1)\frac{d+1}{2}+$ $+(p-d-1)=\frac{d}{2}(\frac{d}{2}-1)+p-\frac{3}{4}$, if d is odd.

The end vertex v has the longest distance among the vertices of the path. Let the remaining vertices $p-d-1$ which are out of the path be located at a distance d from the vertex v. For such a vertex $D(v)=D_{max}$ and $D(v)=\frac{1}{2}(d+1)d+d(p-d-1)=$ $=pd-\frac{1}{2}d(d+1)$.

For the completion of the proof let us show that there are graphs G and H such as $D(v)=D_{min}$, $D(u)=D_{max}$ (Fig. 14). The lemma is proved.

The question arises of how strong could differ the vertex distances from D_{min} and D_{max} for the vertices of the same graph. For vertices u , w in the graph G given in Fig. 14, d is even, $D(u)=D_{max}$ and $D(w)<2D_{min}$ that can be demonstrated by direct calculation.

COROLLARY.
$$\frac{D_{min}}{D_{max}} \geqslant \frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{p}}$$

PROOF. Using the expression for D_{min} and D_{max} from the Lemma 1 we get $\frac{D_{min}}{D_{max}}=\frac{d^2/4-d/2+p-c}{pd-d^2/4-d/2} \geqslant \frac{d^2/4+p/2}{pd}=$

$$=\frac{1}{p}\left(\frac{d}{4}+\frac{p}{2d}\right) \geqslant \frac{1}{2p}\min_d\left(\frac{d}{2}+\frac{p}{d}\right).$$

The expression $\frac{d}{2}+\frac{p}{d}$ achieves its minimal value at $d=\sqrt{2p}$ whence

$$\frac{D_{min}}{D_{max}} \geqslant \frac{1}{2p}\left(\frac{\sqrt{2p}}{2}+\frac{p}{\sqrt{2p}}\right)=\frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{p}}$$

as desired to prove.

THEOREM 4. Let G be a graph of the order p and $v\in V(G)$ then

$$\frac{1}{p} \leqslant \frac{D(v)}{D(G)} \leqslant 2\sqrt{2}\cdot\frac{1}{\sqrt{p}} \quad .$$

PROOF. The lower bound follows from the inequality

$$2D(G)=\sum_{u,v\in V(G)} d(u,v) \leqslant \sum_{u,v\in V(G)} (d(u,w)+d(w,v)) \leqslant 2pD(w).$$

Let $D(w)=\min_{v\in V(G)} D(v)$ then for arbitrary vertex $v\in V(G)$

$$\frac{D(v)}{D(G)} \geqslant \frac{D(w)}{pD(w)}=\frac{1}{p} \quad .$$

To prove the upper bound we use collorary of Lemma 1. We have

$$\frac{D(v)}{D(G)} \leqslant \frac{2D_{max}}{pD_{min}} \leqslant \frac{2}{p}\sqrt{2p}=2\sqrt{2}\,\frac{1}{\sqrt{p}} \quad .$$

The theorem is proved.

Let us give an example of a graph where the ratio $D(v)/D(G)$ is close to the upper bound of the Theorem 4. For the graph G given in Fig. 14 with a diameter $d=\sqrt{p}$ the value $D(w)/D(G)\geqslant\frac{1}{2}\cdot\frac{1}{\sqrt{p}}$ at $p>2$ that can be demonstrated by direct calculation.

For a more detailed description of the subgraph relative position in a graph one can use more complicated characteristics of graphs as, for example, the path characteristics. For hexagonal rings H_1, H_2 in the graph G in Fig. 15 at $V_0=V(G)$ the values of relative distances coincide $D(H_1,V_0)=D(H_2,V_0)=$ $=0.14653$, but the relative path distance values are different

$D_\tau(H_1,V_0)$ = 0.318, $D_\tau(H_2,V_0)$ = 0.409, where $D_\tau(H,V_0) = \frac{1}{D_\tau(G)} \cdot D_{\tau V_0}(H)$.

The relative characteristics can also be used for the definition of the subgraph mutual positions in a graph. Let H_1, $H_2 \subseteq G$, H_1 and H_2 be connected, $V(H_1) \cap V(H_2) = \emptyset$. We will denote the distance $D(H_1,V_0)$ at $V_0 = V(H_2)$ as $D(H_1,H_2)$ .The value $D(H_1,H_2)$ characterizes the position of subgraph H_1 in respect to the subgraph H_2 in graph G . It is clear that $D(H_1,H_2) = D(H_2,H_1)$. Let us consider the graph G in Fig. 16 and the hexagonal rings $H_1, H_2, H_3 \subseteq G$. The relative distances $D(H_1,H_2) = D(H_2,H_3)$ = 0.386 but for the path distances $D_\tau(H_2,H_1)$ = 0.115 and $D_\tau(H_2,H_3)$ = 0.114.

8. BLIND SET OF A GRAPH

Each relative partition $\hat{G}(v), v \in V(G)$ induces the the partition of the graph vertex degrees. Let $u \in V_i(v)$, then the layer $V_i(v)$ we shall call the proper layer for the vertex u and the layers $V_{i-1}(v)$ and $V_{i+1}(v)$ - the left and right adjacent layers, respectively. Then $\deg u = \deg_\ell u + \deg_p u + \deg_r u$ where $\deg_\ell u, \deg_p u, \deg_r u$ denote the number of vertices adjacent to u in the left, proper and right adjacent layers respectively. It is clear that for any vertex u in the partition $\hat{G}(v)$ $\deg_\ell(u) \neq 0$ except for vertex v and for $u \in V_{e(v)}(v)$ $\deg_r u = 0$. In the partition $\hat{G}(v)$ in Fig. 17 $\deg_\ell u = 2$, $\deg_p u = 1$, $\deg_r u = 1$.

The layer $V_{e(v)}(v)$ we shall call the partition shell $\hat{G}(v)$ and the set $S(G) = \bigcup_{v \in V(G)} V_{e(v)}(v)$ - the shell of the graph

G . The vertex u is called the blind vertex for the partition $\hat{G}(v)$ if $\deg_2 u = 0$, $u \neq v$ and the vertex u does not belong to the partition shell. The vertex w will be the blind vertex for the partition $\hat{G}(v)$ in Fig. 17. The set of all the partition blind vertices let us denote as $T(\hat{G}(v))$.

DEFINITION 9. The set $T(G)$ such as $v \in T(G) \Leftrightarrow v \in \bigcap_{u \neq v} T(\hat{G}(u))$ is called the blind set of the graph G .

If $v \in T(G)$, v will be called the blind vertex of the graph G . Let $v \in V(G)$ then the subgraph induced upon the vertex set adjacent to v will be denoted by G_v .

THEOREM 5. Let $\deg v = m$ in the graph G , then

$$v \in T(G) \Leftrightarrow G_v \simeq K_m \text{ and } v \notin S(G) .$$

PROOF. The necessity. Let $v \in T(G)$ and G_v is assumed to be $G_v \not\simeq K_m$. Then in G_v there are nonadjacent vertices u and w . Let us construct the partition $\hat{G}(u)$ (Fig. 18a). In this partition $\deg_2 v \neq 0$, i.e. $v \notin T(G)$. Whence $G_v \simeq K_m$. The condition $v \notin S(G)$ follows from the definition of $T(G)$. The sufficiency. Let $G_v \simeq K_m$ and $v \notin S(G)$. Let us show that in all the relative partitions $\deg_2 v = 0$. Let there be the partition with $v \in V_i$ and $\deg_2 v \neq 0$ (the fragment of the partition is given in Fig. 18b). Then the layers V_{i-1} and V_{i+1} will contain the vertices adjacent to v whence $G_v \not\simeq K_m$. Thus, in all the partitions $\deg_2 v = 0$. The theorem is proved.

The proved theorem enables us to localize the places of probable "location" of vertices from $T(G)$ in the graph G . For the graph given in Fig. 19 $T(G) = \{v_1, v_2, v_3, v_4\}$. The vertex set $v \in V(G)$ such as $e(v) = d(G)$ is called the periphery of the graph G and will be denoted as $P(G)$. Before shifting to considering the set $T(G)$ for various graphs let us formulate the sufficiently evident auxiliary statement.

LEMMA 2. If G is a tree then $v \in S(G) \Leftrightarrow v \in P(G)$.

PROOF. The sufficiency is evident since for any $v \in P(G)$ there exists $u \in P(G)$ such as that $d(u,v) = d(G)$. Consequently v is in the partition shell $\hat{G}(u)$, i.e. $v \in S(G)$. The necessity. Let $v \in S(G)$ and assume that G has a single central vertex u. Let $v \notin P(G)$ that is equivalent to the condition $d(u,v) < r(G)$ where $r(G)$ is the radius of G. Let us consider an arbitrary partition $\hat{G}$ with $u \in V_i$. Since in the tree $deg_\ell u = 1$ and $deg_s u = 0$, then the vertex will be from $P(G)$ laying in the layer $V_{i+r(G)}$. Whence v does not lay in the shell $\hat{G}$ as $d(u,v) < r(G)$ and because of arbitrariness of the partition $\hat{G}$ we have that $v \notin S(G)$. We get the contradiciton whence $v \in P(G)$. For the bicentral trees the proof procedure is similar. The lemma is proved.

COROLLARY 1. The blind set of a tree consists of all the nondiametric pendant vertices.

PROOF. If $v \in P(G)$ where G is a tree then $v \notin T(G)$ since according to Lemma 2 $P(G) = S(G)$. From the Theorem 5 follows that the existence of the nonpendant vertex $v \in T(G)$ in the graph G induces the existence of a cycle in G. Consequently in the tree G the nonpendant vertices cannot belong to $T(G)$. It is left to note that the pendant vertices being nondiametric satisfy the conditions of the Theorem 5. The corollary is proved.

COROLLARY 2. If in the tree G $d(G) < 4$ then $T(G) = \emptyset$.

PROOF. For the tree G with a diameter $d(G) \leqslant 3$ the set $P(G)$ coincides with the set of all pendant vertices whence according to the Corollary 1 $T(G)=\emptyset$. The corollary is proved.

Fig. 20 shows the tree G where $d(G)=4$ and $T(G)=\{v\}$.

COROLLARY 3. If in the graph G $d(G)<3$ then $T(G)=\emptyset$.

PROOF. If $r(G)=d(G)=1$ or $r(G)=d(G)=2$ then $V(G)=P(G)$ whence $T(G)=\emptyset$ since $P(G)\subseteq S(G)$. Let $r(G)=1$, $d(G)=2$ and the vertices $u, v\in V(G)$ be as that $e(v)=1, e(u)=2$. Then in the partition $\hat{G}(u)$ $\deg_r v\neq 0$ and $u\in P(G)$. Consequently, $T(G)=\emptyset$. The corollary is proved.

Fig. 21 shows the graph G where $d(G)=3$ and $T(G)=\{v\}$.

COROLLARY 4. If G is a regular graph then $T(G)=\emptyset$.

PROOF. Let the graph G vertices of the order p have a degree m. Let us assume that $v\in T(G)$. According to the Theorem 5 $G_v\simeq K_m$ and in G $\langle V(G_v)\cup v\rangle \simeq K_{m+1}$. Since, according to the Corollary 3, $T(K_{m+1})$ then $\exists u$ $\deg u>m$, whence G is not a regular graph of a degree m. This is a contradiction. Consequently, for a regular graph G $T(G)=\emptyset$. The corollary is proved.

The following statements concern some extreme properties of graphs with the blind sets.

THEOREM 6. Let in the graph G $T(G)=\emptyset$ then the minimal order p of the graph G is equal to

$$p=\begin{cases} 6, & \text{if } G \text{ is a tree,} \\ 5, & \text{in other cases} \end{cases}$$

PROOF. Let G be not a tree. From the Corollary 3 follows that for the graph G its minimal diameter $d(G)=3$ whence $p\geqslant 5$. The graph in Fig. 21 has the order $p=5$ and $T(G)=\{v\}$. If is a tree then according to the Corollary 2 the minimal diameter of G $d(G)=4$. As $T(G)$ consists of the pendant nondiametric vertices (Corollary 1 of the Theorem 5), $p\geqslant 6$. The tree in Fig. 20 has the order $p=6$ and $T(G)=\{v\}$. The theo-

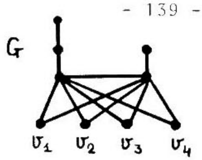


Fig. 19

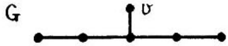


Fig. 20

Fig. 21

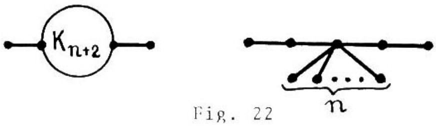


Fig. 22

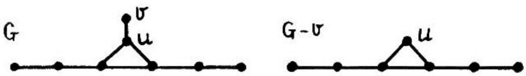


Fig. 23

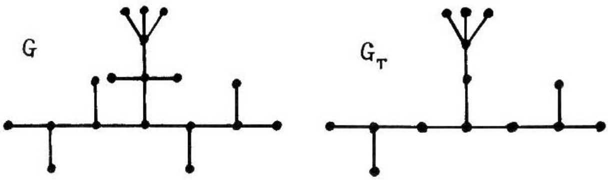


Fig. 24

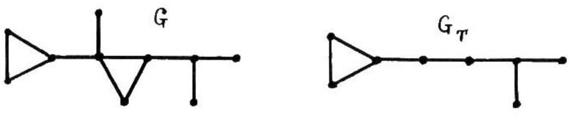


Fig. 25

rem is proved.

COROLLARY. Let in the graph G $|T(G)|=n$ then the minimal order p of the graph G is equal to

$$p=\begin{cases} n+5, & \text{if } G \text{ is a tree,} \\ n+4, & \text{in other cases.} \end{cases}$$

PROOF. The minimal order of graphs for which $|T(G)|=1$ is determined by the Theorem 6. To the graphs in Figs. 20 and 21 let us add $n-1$ vertices in such a way that in a new graph they could belong to $T(G)$. Such graphs are given in Fig. 22. The corollary is proved.

Let $Y(G)$ be a set of cut points of the graph G.

THEOREM 7. $T(G) \cap Y(G) = \emptyset$

PROOF. Let $v \in T(G)$. As in all the relative partitions $\deg_\tau v = 0$ then with deleting the vertex v for any vertex u $\deg_\tau u \neq 0$. Consequently, after the deletion of v the graph G is remained to be connected, i.e. $v \notin Y(G)$. The theorem is proved.

The deletion of the graph blind vertices does not influence the graph metric properties since the distance between the remained vertices is conserved. If $v \in V(G)$ then $G-v$ will denote the graph obtained from G by deleting the vertex v and its incident edges.

THEOREM 8. If $v \in T(G)$ then

1) For any vertex $u \in V(G-v)$ $e_G(u) = e_{G-v}(u)$, in particular $\tau(G)=\tau(G-v)$ and $d(G)=d(G-v)$.

2) For any vertex $u,w \in V(G-v)$ $d_G(u,w) = d_{G-v}(u,w)$.

PROOF. From the Theorem 7 it follows that $G-v$ is connected. As in all the relative partitions of the graph G $\deg_\tau v = 0$, then in the corresponding partitions of the graph $G-v$ all the vertices will belong to the layers with the same number as those in the partitions of G. Consequently, the distances between vertices in $G-v$ will be the same as those in G. The theorem is proved.

The graphs in which the deletion of any vertex causes the change in a parameter based on the vertex distances we shall call the vertex-critical graphs. Well known are such particular cases of the vertex-critical graphs as the vertex-critical graphs upon either diameter or radius [19,20].

COROLLARY. If $T(G) \neq \emptyset$ then G is not a vertex-critical graph.

PROOF. Let $v \in T(G)$ then with the deletion of the vertex according to the Theorem 7 $G-v$ will be connected and by the Theorem 8 the distance between vertices in $G-v$ does not change. The corollary is proved.

Let us consider how the graph metric characteristics are changed with the deletion of the graph blind vertex.

THEOREM 9. If $v \in T(G)$ then $D(G) = D(G-v) + D(v)$, $e(G) = e(G-v) + e(v)$.

PROOF. Using the Theorem 8 we get $2D(G) = \sum\limits_{u \in V(G)-v} D_G(u) +$

$$+ D(v) = \sum_{u \in V(G)-v} \Big(\sum_{x \in V(G)-v} d_G(u,x) + d_G(u,v)\Big) + D(v) =$$

$$= \sum_{u,x \in V(G)-v} d_G(u,x) + \sum_{u \in V(G)-v} d_G(u,v) + D(v) = \sum_{u,x \in V(G)-v} d_{G-v}(u,x) +$$

$$+ 2D(v) = 2D(G-v) + 2D(v).$$

Analogous to it $e(G) = \sum\limits_{u \in V(G)-v} e_G(u) + e(v) =$

$$= \sum_{u \in V(G)-v} e_{G-v}(u) + e(v) = e(G-v) + e(v).$$

The theorem is proved.

Let us consider the properties of graphs obtained with the deletion of the blind vertices.

DEFINITION 10. The nonblind subgraph of the graph G is called the subgraph $G_T \subseteq G$ of maximal order such as that $T(G_T) = \emptyset$.

Let us note that with the deletion of $v \in T(G)$ from the graph G the condition $u \in T(G-v)$ can be satisfied for the vertex $u \notin T(G)$ as shown in Fig. 23 where $v \in T(G)$, $u \notin T(G)$ and $u \in T(G-v)$. The construction of the graph G_T consists in the following: all vertices $T(G)$ are deleted from the graph G; from the graph obtained G_1 all the vertices $T(G_1)$ are deleted, etc.

THEOREM 11. For any tree G there exists a single nonblind subgraph G_T consisting of diametric paths.

PROOF. According to the Corollary 1 of the Theorem 5 $T(G)$ consists of nondiametric pendant vertices. Since upon the deletion of $T(G)$ a new graph will also be a tree, the pendant vertices in G_T will only be diametric ones. The theorem is proved.

Fig. 24 shows a tree G and its G_T .

THEOREM 12. For an arbitrary graph G there exists the single nonblind subgraph G_T .

PROOF. Let G_1 and G_2 be the graphs obtained from G by the deletion of vertices $T(G)$ but the vertices are deleted in different successions. According to the Theorem 8, with the deletion of the blind vertex all the distances between vertices remained are conserved and since $V(G_1) = V(G_2)$, then G_1 and G_2 have the same distance matrix, whence $G_1 \simeq G_2$. From the way of construction of G_T follows the uniqueness of G_T . The theorem is proved.

COROLLARY. For the graph G the subgraph G_T has the order of not less than $d(G)+|P(G)|-1$.

PROOF. Since, according to the Theorem 8, the graph diameter does not change after the deleting its blind vertices and the diametric vertices cannot be the blind ones, the order of G_T cannot be less than $d(G)+|P(G)|-1$. The corollary is proved.

For the graph G in Fig. 25 the subgraph G_T has an order equal to $d(G)+|P(G)|-1$. It is evident that $G \simeq G_T \Leftrightarrow T(G)=\emptyset$. From the previous considerations it follows that G_T conserves the metric properties of G, i.e. for any vertex $u \in V(G_T)$ $e_{G_T}(u)=e_G(u)$ and for any $u,v \in V(G_T)$ $d_{G_T}(u,v)=d_G(u,v)$.

THEOREM 13. If G is a tree and $d(G)>3$ then $T(\bar{G})=\emptyset$.

PROOF. Since $d(G)>3$ then $\bar{G}$ is connected and from the property of a tree it follows that $d(\bar{G})=2$. According to the Corollary 3 of the Theorem 5 for the graphs with such a diameter the blind set is empty $T(G)=\emptyset$. The theorem is proved.

The graph G in Fig. 21 is a selfcomplimentary and $T(G)=$ $=T(\bar{G})=\{v\}$. For G in Fig. 26 $T(G)=\emptyset$ but $T(\bar{G})=\{u_7\}$.

THEOREM 14. If $|T(G)|=n$ then $T(G)=\bigcup\limits_{i=1}^{t} K_{p_i}$, where $p_1+p_2+\ldots+p_t=n$ and $1 \le p_i \le n$, $i=1,2,\ldots,t$.

The proof follows from the Theorem 5.

Fig. 27 shows the graph G for which $T(G)=K_1 \cup K_2 \cup K_3 \cup K_1$.

COROLLARY. If G is the selfcomplimentary graph, $T(G)\neq\emptyset$ and $T(G)=T(\bar{G})$ then $|T(G)|=1$.

PROOF. Let $|T(G)|=n$. Since $G \simeq \bar{G}$ and $T(G)=T(\bar{G})$ then $\langle T(G)\rangle \simeq \overline{\langle T(G)\rangle}$ is satisfied. According to the Theorem 14 this is equivalent to the condition $\bigcup\limits_i K_{p_i} \simeq \overline{\bigcup\limits_i K_{p_i}}$ which, as is

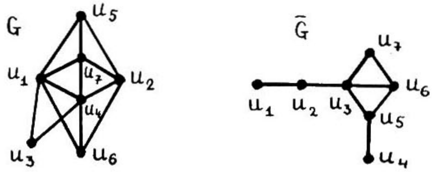


Fig. 26

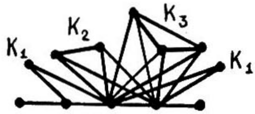


Fig. 27

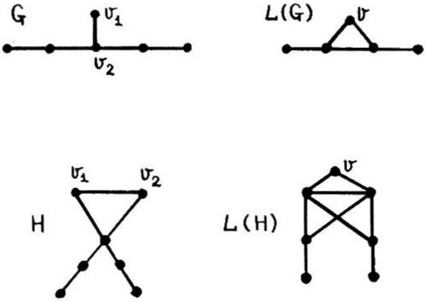


Fig. 28

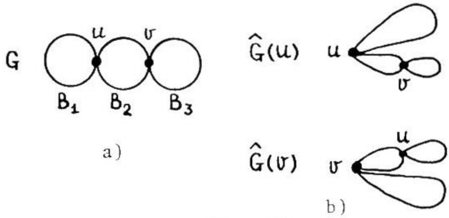


Fig. 29

easy to verify, is satisfied only at $n=1$. The corollary is proved.

Let $L(G)$ detone the line graph for the graph G .

THEOREM 15. If G is a biconnected then $T(L(G))=\emptyset$.

PROOF. Let the edge (v_1,v_2) of the graph G correspond to the vertex $v\in V(L(G))$. The vertex v can belong to $T(L(G))$ only under the condition that one of the following conditions is satisfied:

1. the edge (v_1,v_2) is incident to the pendant vertex G ,
2. the edge (v_1,v_2) belongs to the triangle in G and $\deg v_1=\deg v_2=2$.

Really, since in $L(G)$ for the vertex v of the degree m should be satisfied the condition $G_v\simeq K_m$ then in G all the edges incident to the edge (v_1,v_2) should be incident to each other. This is only possible if one of the mentioned above conditions is satisfied. Note, that one of the conditions for 1) or 2) to be satisfied is the condition $Y(G)\neq\emptyset$ whence follows the theorem statement. The theorem is proved.

For the graphs G and H in Fig. 28 edge (v_1,v_2) corresponds to the blind vertex v of the line graphs.

9. FLAT GRAPHS

Let us consider the graphs in any relative partition of which there is not blind vertices.

DEFINITION 11. The graph G is called flat if $\bigcup\limits_{v\in V(G)} T(\hat{G}(v))=\emptyset$.

The main property of the flat graphs is that for any vertex u in any relative partition (u does not belong to the shell) $\deg_z u\neq 0$.

THEOREM 16. The flat graph has not more than one cut point.

PROOF. Let the vertices u and v be the cut points of the graph G then G consists of not less than three blocks B_1, B_2, B_3, (Fig. 29a). Denote $K_1 = \max\limits_{w \in V(B_1)} d(u,w)$, $K_2 = d(u,v)$, $K_3 = \max\limits_{w \in V(B_3)} d(v,w)$. Let us construct the relative partition $\hat{G}(u)$ and $\hat{G}(v)$ whose diagrams are given in Fig. 29b. From the condition of G flatness follows that $K_1 = K_2 + K_3$ and $K_3 = K_2 + K_1$ whence $K_1 = K_3$ and $K_2 = 0$. Consequently, the vertex u coincides with v and G has the only cut point. If G consists of many blocks, the proof procedure is similar. The theorem is proved.

As an example of the flat graph with the cut point is a star $K_{1,p-1}$. Examples of some flat graphs - complete graph K_p, complete m-part graph $K_{p_1,p_2,\dots,p_m}$, wheel W_p, graphs of a diameter 2 without triangles, p-dimensional cube Q_p, simple cycle C_p, Moore's graphs.

The properties of flat graphs can be used for the study of metric characteristics.

THEOREM 17. If for the flat graph G of the order p the shell of every partition has one vertex then $D(G) = \frac{p}{4} e(G)$.

PROOF. Let us consider the partition $\hat{G}(v)$ and let the vertex u belong to the shell. Since G is flat then for any vertex $w \in V(G)$

$$d(v,w) + d(w,u) = e(v) = e(u) = \frac{1}{2}(e(v) + e(u)) \qquad (*)$$

Summing (*) over all $w \in V(G)$ we have $D(v) + D(u) = \frac{p}{2}(e(v) + e(u))$. Summing both parts of this equality over all various pairs $\{u,v\}$ we get $D(G) = \frac{p}{4} e(G)$. The theorem is proved.

Some examples of graphs satisfying the conditions of the Theorem 16 one can find out in Ref. [21].

C O N C L U S I O N

In this work some directions of studies of metric properties of graphs were considered. An analysis of metric properties of graphs is based on the concept of relative partitions and corresponding layer matrix of a graph. Metric characteristics of graphs find their application in chemical research, for example, in the problem of construction of topological indices of molecular graphs. An application of the relative characteristics can be substantiated by the fact that the properties of chemical compounds not only depend on the presence of some fragment in the compound but also on the fragment position in the molecule, on the mutual disposition of fragments, on the form of the molecule itself. The relative metric characteristics enable one to distinguish the embeddings of the same fragment in the molecular graph, to characterize the interconnection of fragments in a molecule. The use of the path characteristics permits to take into account more completely the structural features of graphs. The layer matrix and path layer matrix of a graph enables one to use the common method for calculating the metric and path characteristics and also some relative characteristics. The well known topological indices as the Wiener number and others [1] can easily be obtained with the corresponding matrices.

The problems of identification of graphs with the layer matrix of various orders, complete layer matrix (together with the edge part) are investigated in the work. Of interest is the study of a possibility to identify graphs with a path layer matrix. Some examples of nonisomorphic graphs of the order 18 which are not the trees with the same path laver matrices are presented in the work. These examples give a negative answer to the assumption formulated in Ref. [18]. Still open is the question of whether there are nonisomorphic graphs of the order p, $12 \leq p \leq 17$ having the same path layer matrix.*)

Considered in the work are the graph correspondences conserving the distances. The criterion of existence for isometric correspondence is formulated in terms of the layer matrix. The existence criterion for isotopic correspondence is a more complicated one - coincidence of the paired different line sets of path layer matrices is only the necessary condition for the existence of correspondence conserving the path distance.

The graph blind vertices were considered which deletion from the graph does not change the mutual distances between the vertices remained. The conditions are obtained for the existence of the blind vertices in a graph, the blind vertex properties are studied for various classes of graphs.

Note, that the work presented here could not cover the other porblems of metric analysis. For example, for the Wiener number theory it is of interest to study the regularities in changes of a graph distance under some structural transformation, the concept of structural isotopicity (the graph correspondence conserving the structure of paths outgoing from vertices) was not considered.

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*) As follows from the latest results this question is left open for graphs of the order p, $12 \leq p \leq 13$. The problem from Refs. [3,18] on the existence of nonisomorphic regular graphs of a degree τ with coinciding path layer matrices is solved for any $\tau \geq 3$, the orders of such graphs are defined.

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