Embeddings of Chemical Graphs in Hypercubes

M. Deza and M. I. Shtogrin

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Abstract. We study planar graphs embedded in the plane that have chemical applications: the degrees of all vertices are 3 or 2, all internal faces but one or two are r-gons, and each internal face is a simply connected domain. For wide classes of such graphs, we solve the existence problem for embeddings of the graph metric on the vertices in multidimensional cubes or cubical lattices preserving or doubling all the distances. Incidentally we present a complete classification of some interesting families of such graphs.

Key words: chemical graphs, plane graphs, graph metric, metric preserving embeddings of graphs in hypercubes, pericondensed and catacondensed graph, 3-connected graph, polycycle.

The present paper is devoted to the study of simply connected polygonal systems. These are plane graphs formed by the boundaries of polygons (from now on these polygons will be called internal faces) filling a connected simply connected domain and such that any two polygons either do not intersect, or intersect in an edge. It follows that the valency of each vertex of the graph lying inside the domain equals 3, while the valency of each vertex on the boundary of the domain is either 2 or 3. In organic, physical, and mathematical chemistry such graphs represent polycyclic conjugate hydrocarbons and polycyclic aromatic hydrocarbons. The simple connectedness of the domain forbids any holes in it (hence, we exclude, e.g., coronoids); in chemical terms, we consider fully condensed polycyclic aromatic hydrocarbons C_nH_m, where n is the total number of vertices (carbon atoms C), and m is the number of vertices of valency 2 (hydrogen atoms H). In chemistry, a graph is called peri- or catacondensed depending on whether it contains vertices that are internal points of the domain. By the Steinitz theorem, a finite 3-connected chemical graph C_nH_0 always is the edge-skeleton of a polyhedron. However, we shall be concerned mainly with graphs having vertices of valency 2 as well, i.e., with the case of a nonzero number of hydrogen atoms.

A chemical graph together with all its internal faces is called a *polycycle* (or, to be more precise, a *poly-r-cycle*) if all internal faces are combinatorial r-gons. The r-cycles of a given polycycle are its minimal cycles (see [1]). A graph is called a *mono-q-r-cycle* if all its internal faces but one q-gon are r-gons.

Finally, a *di-q-r-cycle* is a graph having two q-gons and a number of r-gons as its internal faces. These three classes cover most of the chemical graphs studied in the chemical literature (see, e.g., [2–5] and numerous references there; our chemical terminology is borrowed from these references).

In Fig. 1 the reader can find examples of chemical graphs, prototypes of the corresponding series.

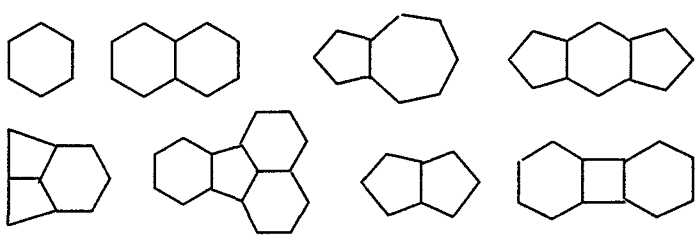

Fig. 1. Examples of chemical graphs: benzene C_6H_6, naphtalene $C_{10}H_8$, azulene $C_{10}H_8$, indancene $C_{12}H_8$, terphenylenoid C_9H_5, fluoranthene $C_{16}H_{10}$, pentalene C_8H_6, biphenylene $C_{12}H_8$

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The problem we study here is to find all graphs in a given class of chemical graphs that admit an *embedding* in a hypercube $\mathbb{H}_d$ or a half-cube $\frac{1}{2}\mathbb{H}_d$, $d \le \infty$. Namely, we are interested in whether it is possible to associate to each vertex of a graph a binary sequence of length d so that the distance between any two vertices in the graph is equal either to the Hamming distance between the corresponding sequences, or to half the Hamming distance (the scale must be the same for all distances, see [6]). A polynomial algorithm checking the existence of such an embedding is presented in [7]. Approaches to the search for such embeddings are suggested in [6] and [8].

In mathematical terms, a graph is embeddable in a hypercube (with a given scale) iff there is an isometric embedding of the graph in the space l_1^k. In mathematical chemistry, such embeddings were studied only for benzenoids [9]. Theorem 3 provides a wide extension of this result including all poly-6-cycles. It is explained in [9] why such embeddings are interesting for chemists: they are convenient for computing parameters depending on the distances (the Wiener number, i.e., the sum of all pairwise distances in a graph, and so on), as well as for ranging purposes.

A simply connected poly-6-cycle has two more names: a *fusene* and a *polyhex*. Such a graph is also called a *benzenoid* or a *helicene* depending on whether it is a subgraph of the hexagonal partition (6^3) of the plane or not. By analogy, we call an r-*helicene* for $r = 3, 4, 5$, $r \ge 7$ a poly-r-cycle which is not a proper subgraph of the edge skeleton of the tetrahedron, the cube, the dodecahedron, or the partition of the Lobachevski plane into r-gons with three edges meeting at each vertex, i.e., of the partition (r^3), respectively. Each r-helicene admits a continuous locally homeomorphic cellular mapping into (r^3) (see [1]).

We call a poly-r-cycle *proper* if it is not an r-helicene, i.e., if it is a proper subgraph of the regular partition (r^3) of the sphere for $r = 3, 4, 5$, of the Euclidean plane for $r = 6$, and of the Lobachevski plane for $r \ge 7$. All improper poly-r-cycle are r-helicenes. A proper poly-r-cycles can be an isometric subgraph of the partition (r^3) or not. In the first case such graph is embeddable; in the second case both possibilities are realized. For example, there are precisely $1 + 1 + 3 + 7 + 23$ poly-6-cycles with $p_6 = 1, 2, 3, 4, 5$. All of them are proper, the first helicene arises for $p_6 = 6$. Precisely 8 of these 35 poly-6-cycles are not isometric to a subgraph in (6^3): the one in Fig. 2a, six of its extensions in the edges c, f, g, h or in the pairs of edges $(a, b), (d, e)$, and the one in Fig. 2b. Note that all finitely embeddable poly-r-cycles are embeddable in $\mathbb{H}_{d/2}$ if r is odd, and in $\frac{1}{2}\mathbb{H}_d$ if r is even (here if there are no closed domains bounded by inner edges, d is the perimeter of the covered domain, i.e., the length of the boundary of the external face).

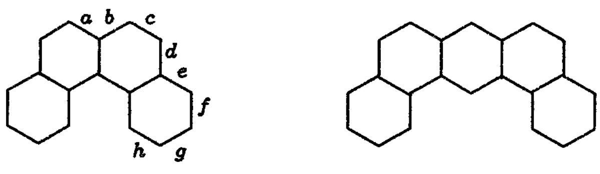


FIG. 2. All pairwise nonisomorphic subgraphs of (6^3) with $p_6 \le 5$

Before starting the proof, let us introduce the required tools and notions. The notation $G \to \mathbb{H}_d$, $G \to \frac{1}{2}\mathbb{H}_d$, $G \to \mathbb{Z}_d$, $G \to \frac{1}{2}\mathbb{Z}_d$, $d \le \infty$, means that the graph G endowed with the scale $\lambda = 1$ or $\lambda = 2$ is embeddable in the cube $\mathbb{H}_d$, or (if the graph is infinite) in the cubical lattice $\mathbb{Z}_d$; the coefficient $\frac{1}{2}$ means that the embedding doubles all distances between the vertices. Further, $G - e$, $G - v$ denotes the graph obtained from G by erasing an edge or a vertex; $P_n, P_{\mathbb{N}}, P_{\mathbb{Z}}$ denotes an edge path whose vertices are either $\{1, 2, \dots, n\}$, or $\mathbb{N}$ (positive integers), or $\mathbb{Z}$ (all integers) respectively; $G \times G'$ is the direct (Cartesian) product of the graphs G and G'; $\alpha_3, \beta_3, \gamma_3$, Do and Ico denote respectively the tetrahedron, the octahedron, the cube, the dodecahedron, and the icosahedron (and their 1-skeletons if we speak about graphs).

An important necessary condition of the embeddability of a graph is its 5-gonality [10]: for any five vertices x, y, a, b, c of the graph the 5-*gonal inequality*

$$\rho_{xy} + (\rho_{ab} + \rho_{ac} + \rho_{bc}) \le (\rho_{xa} + \rho_{xb} + \rho_{xc}) + (\rho_{ya} + \rho_{yb} + \rho_{yc}) \qquad (*)$$

must be satisfied. In all examples for which we prove that a graph is not embeddable, we point out five vertices contradicting this requirement. In the figures, vertices a, b, c are marked by circles, and vertices x, y are marked by squares.

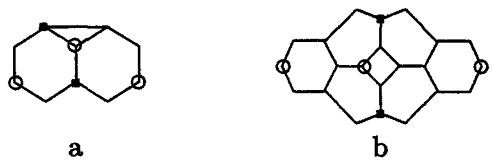


FIG. 3. Forbidden isometric subgraphs of embeddable mono-3- and mono-4-fusenes.

The class of graphs we study here is, in a sense, opposite to the class of planar graphs with valencies of all internal vertices greater than 3 and not containing triangles: such graphs are embeddable, as it is proved in [11]. Note that a graph consisting of the triangle, an m-gon, and an n-gon meeting at a vertex of valency 3 is embeddable iff both m and n are odd, see [12]; Figure 3a illustrates verticies violating 5-gonal inequality $(*)$ for $m = n = 6$.

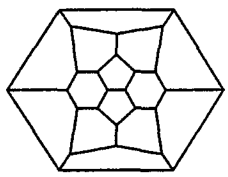


FIG. 4. Fullerene $F_{26} \to \frac{1}{2}\mathbb{H}_{12}$. The central subgraph $\Gamma_{1,1}$ is neither 5-gonal, nor isometric

The uniform partitions $(6^3) \to \mathbb{Z}_3$, $(4.8^2) \to \mathbb{Z}_4$, $(4.6.12) \to \mathbb{Z}_6$, the non 5-gonal partition (3.12^2) of the Euclidean plane, as well as the uniform partitions $(r^3) \to \mathbb{Z}_\infty$ for r even and $(r^3) \to \frac{1}{2}\mathbb{Z}_\infty$ for r odd provide examples of simply connected polygonal systems. Of course, the following polyhedra taken without one face also satisfy the definition: $\alpha_3 \to \frac{1}{2}\mathbb{H}_4$, $\gamma_3 \to \mathbb{H}_3$, Do $\to \frac{1}{2}\mathbb{H}_{10}$, the truncated octahedron is embeddable in $\mathbb{H}_6$, as well as the non 5-gonal truncated polyhedra α_3, γ_3, Do and Ico. Figure 4 shows, as an example, the graph of the fullerene $F(26)$ (a polyhedron with vertices of valency 3 having 12 five-gonal and 3 six-gonal faces) embeddable in $\frac{1}{2}\mathbb{H}_{12}$. This example also is interesting from the following points of view: it has nonalternated zones (see the definition before Theorem 2), and the non 5-gonal subgraph $\Gamma_{1,1} = C_{14}H_8$ introduced in Remark 4 (ii) and shown in Fig. 5b is here a nonisometric subgraph of the embeddable fullerene shown in Fig. 4.

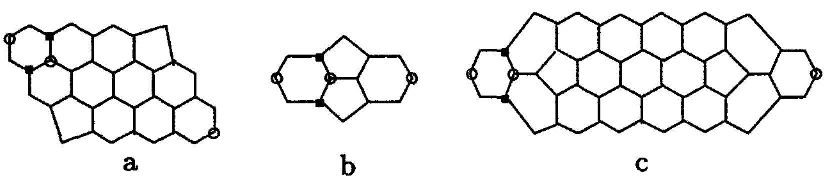


FIG. 5. Forbidden isometric subgraphs of embeddable di-5-fusenes

Similarly to the case of polygons, the main parameter describing plane graphs under consideration is the *p-vector* $p = (p_3, p_4, \dots)$, where p_i is the number of combinatorial i-cycles, i.e., the number of i-gons among the internal faces.

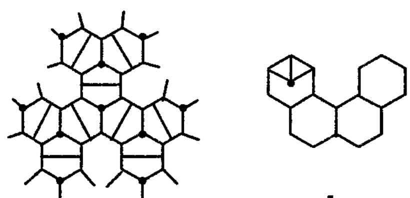
In the present paper, we study the following nine cases:

1) poly-3-cycles: p_3 is arbitrary, all other $p_i = 0$;
2) poly-4-cycles: p_4 is arbitrary, all other $p_i = 0$;

3) poly-5-cycles: they are introduced in [2];
4) $p_3 = p_4 = 0$, $p_5 \leq 1$, all other p_i are arbitrary;
5) mono-3-6-cycles: $p = (p_3 = 1,\ p_6)$;
6) biphenylenoids: $p = (p_4 = 1,\ p_6)$;
7) di-3-6-cycles: $p = (p_3 = 2,\ p_6)$;
8) terphenylenoids: $p = (p_4 = 2,\ p_6)$;
9) indancenoids: $p = (p_5 = 2,\ p_6)$.

Theorem 1 gives a complete description of cases 1) and 2). Theorem 2 presents the list of all forbidden isometric subgraphs of an embeddable poly-5-cycle, i.e., it covers case 3). Theorem 3 guarantees the embeddability for a wide class of chemical graphs relating to case 4). This case includes, for example, poly-6-cycles and azulenoids $p = (p_5 = 1,\ p_7)$. The embeddability of benzenoids, i.e., fusenes that are isometric subgraphs in (6^3) in hypercubes was proved in [9]. Theorem 4 describes all embeddable mono-q-fusenes $(q = 3, 4, 5)$, i.e., cases 5) and 6), as well as embeddable di-3-fusenes, i.e., case 7). Theorem 5 formulates some necessary embeddability conditions for di-q-fusenes with $q = 4, 5$, or, to be more precise, it contains the list of forbidden isometric subgraphs in cases 8) and 9) (there are infinitely many of them). We conjecture that the assumptions of Theorem 5 are not only necessary, but also sufficient for embeddability of terphenylenoids and indancenoids. Finally, Theorem 6 presents the list of all monohedral polypentagons.

All planar graphs without internal vertices (i.e., catacondensed graphs) are embeddable (see [6, Proposition 3]). Moreover, the characterization of embeddable poly-5-cycles and di-5-fusenes by means of forbidden subgraphs shows that any such graph having precisely one internal vertex is embeddable. Each poly-5-cycle with pairwise isolated internal vertices (i.e., no two internal vertices can be connected by an edge path consisting only of internal points) is embeddable; if the number of isolated internal vertices is infinite, then such graph is embeddable in $\frac{1}{2}\mathbb{Z}_\infty$ (see the infinite graph in Fig. 6a). On the other hand, there are nonembeddable di-3-fusenes (i.e., di-3-6-cycles) with a single internal vertex (see Fig. 6b).



a b

FIG. 6. Examples of pericondensed graphs: a) $\rightarrow \mathbb{Z}_\infty$; b) non 5-gonal

Proving the embeddability of graphs below, we make use of the sufficient embeddability conditions for a planar graph given in [6, Proposition 2]. Namely, suppose that the set of edges of a graph splits into zones (sequences of opposite edges of faces alternating directions in the case of odd faces) so that each zone corresponds to the dimension of the cube in which the graph is embedded. Zones mark the edges (by one or two dimensions depending on whether the graph is embeddable or not). Then, picking one of the vertices for the origin, we can mark all the other vertices by the symmetric differences of marked edges on a shortest path starting at the origin. Since the domain filled by internal faces of the graph is simply connected, this marking is independent of the choice of the path connecting the vertex with the chosen origin. Such mapping will be symmetric if the cut corresponding to any alternating zone is convex (see [6]).

Theorem 1. (i) *Here is the list of all poly-3-cycles:* α_3, $(\alpha_3 - e) \rightarrow \frac{1}{2}\mathbb{H}_4$ *(the nonisometric subgraph of the tetrahedron* α_3*)*, $(\alpha_3 - v) = \alpha_2$.

(ii) *Here is the list of all poly-4-cycles:* γ_3, $(\gamma_3 - e)$ *(this graph is not 5-gonal)*, $(\gamma_3 - v) \rightarrow \mathbb{H}_3$, $(P_2 \times P_n) \rightarrow \mathbb{H}_n$, $(P_2 \times P_{\mathbb{N}}) \rightarrow \mathbb{Z}_2$, $(P_2 \times P_{\mathbb{Z}}) \rightarrow \mathbb{Z}_2$. *Subgraphs of the cube:* γ_3, $(\gamma_3 - v)$, $(P_2 \times P_n)$ *for* $n = 2, 3, 4$; *in this list the following graphs are isometric:* γ_3, $(\gamma_3 - v)$, $(P_2 \times P_2) = \gamma_2$, $(P_2 \times P_3)$.

The proof is a direct verification.

Remark 1. There are $1+1+2+4+7+18$ poly-5-cycles with $p_5 = 1, 2, 3, 4, 5, 6$. The following classes of these 33 poly-5-gons are useful.

(i) One graph with $p_5 = 5$ and seven graphs with $p_5 = 6$ are 5-helicenes (i.e., polypentagons that are not subgraphs of the dodecahedron); these are the graph in Fig. 7a, four of its extensions in the edges e, f or in the pairs of edges (a, b), (c, d); three others are shown in Fig. 7b, 7c, 7d (all of them are embeddable).

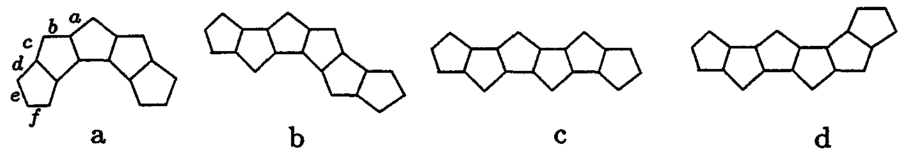


FIG. 7. 5-helicenes with $p_5 \leq 6$

(ii) Precisely five of these 33 graphs are isometric subgraphs of the dodecahedron: G_1, the edge skeleton of the single 5-gon (i.e., the cycle C_5), G_2, the edge skeleton of two 5-gons attached by an edge, G_3, the edge skeleton of three 5-gons of the dodecahedron meeting at a vertex, G_4, the edge skeleton of four 5-gons of the dodecahedron incident to an edge of the dodecahedron, G_5, the edge skeleton of six 5-gons of the dodecahedron with five of them incident to the sixth one. In other words, a subgraph of the dodecahedron is isometric iff it contains no boundary edge incident to three 5-gons. Moreover, these five graphs are all nontrivial isometric subgraphs of the dodecahedron; of course, all of them are embeddable.

(iii) This list of 33 graphs contains precisely two nonembeddable graphs (non 5-gonal configurations are shown in Fig. 8).

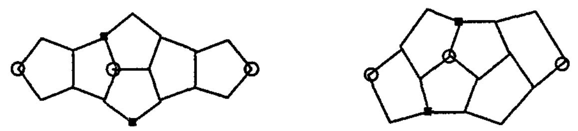


FIG. 8. Forbidden subgraphs of embeddable poly-5-cycles

(iv) All poly-5-cycles that are subgraphs of the dodecahedron are listed in [2, Figs. 3–5].

There are precisely four embeddable subgraphs of the dodecahedron among the remaining fourteen (satisfying $7 \leq p_5$) [2, Fig. 5]: the three nonisometric subgraphs $C_{20}H_8 \to \frac{1}{2}\mathbb{H}_{17}$, $C_{20}H_8 \to \frac{1}{2}\mathbb{H}_{17}$, $C_{19}H_7 \to \frac{1}{2}\mathbb{H}_{15}$, see Fig. 9, and the edge skeleton of Do itself.

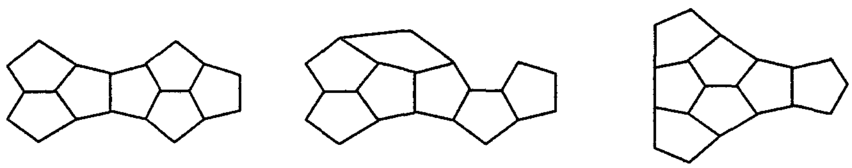


FIG. 9. All embeddable nonisometric subgraphs of the dodecahedron with $p_5 \geq 7$

(v) The edge skeleton of Do has two special subgraphs (that are nonisometric and nonembeddeble): $\mathrm{Do} - v \subset \mathrm{Do} - e \subset \mathrm{Do}$, and this inclusion is the only possible extension of these subgraphs; the graph itself is not a subgraph of any other polycycle.

Remark 2. (i) An example of a poly-5-cycle embeddable only in $\frac{1}{2}\mathbb{Z}_\infty$ is given by the infinite strongly connected chain of 5-gons, which is the universal covering of the finite closed chain of 5-gons consisting of five 5-gons surrounding a 5-gon; this graph, as well as the graph shown in Fig. 6a, contains a tree with an infinite number of edges.

(ii) Any simply connected poly-5-cycle containing not more than one vertex of valency 2 is infinite.

iii) If a poly-r-cycle with $r \geq 6$ has not more than $r-1$ vertices of valency 2, then it is infinite. For $r = 3, 4, 5$ each of the finite-r-cycles $\alpha_3 - e, \gamma_3 - e$, Do $-e$ has two vertices of valency 2, and each of $\alpha_3 - v, \gamma_3 - v$, Do $-v$ as three vertices of valency 2. For $r \geq 5$ there are infinite poly-r-cycles having an arbitrary number of vertices of valency 2.

Below we shall also need the following two definitions.

We denote the polypentagon, i.e., the poly-5-cycle corresponding to a graph G, by $\Pi(G)$. (Essentially, $\Pi(G)$ is the face partition of the disk with the edge skeleton G. It turns out (see [1, 13] and [14]) that the abstract structure of a polypentagon $\Pi(G)$ is uniquely determined by the abstract structure of the graph G. Therefore, we often use the term polycycle for the graph G itself.) Connect a pentagon in $\Pi(G)$ with any other pentagon in this polypentagon by a sequence of pentagons such that our pentagons are the first and the last one in the sequence, and any two successive pentagons in the sequence have a common edge. The *k-neighborhood* of a given pentagon is the union of all pentagons from $\Pi(G)$ admitting a chain of pentagons of length not greater than $k+1$ connecting it with the given one. Then the 0-neighborhood of a pentagon consists of itself, the 1-neighborhood includes the pentagon itself and those pentagons that have a common edge with it, the 2-neighborhood consists of the pentagon iteslf, its neighbors, and neighbors of its neighbors. In particular, the 1-neighborhood of a pentagon in $\Pi(G)$ having precisely five neighbors is $\Pi(G_5)$ (see Remark 1(ii)).

Each edge of a plane n-gon has one opposite edge if n is even, and it has two opposite edges (the left and the right one) if n is odd. A *zone* of a partition of the plane is a sequence of edges (possibly closed) such that each edge in this sequence is opposite to the previous one. A zone is called *alternating* if the corresponding choices of the left and of the right opposite edges alternate.

Theorem 2. *A poly-5-cycle G not coinciding with* Do *is embeddable in $\frac{1}{2}\mathbb{H}_d$ (where d is the perimeter) iff it does not contain subgraphs shown in Fig. 8 (not always isometric).*

We prove the nonembeddability of the graphs in Fig. 8 by picking 5 vertices in each of them violating the 5-gonal inequality. Any isometric subgraph, but not each nonisometric subgraph, violates this inequality. In the last case the 5-gonal inequality can be violated by another choice of the five vertices, different from that shown in Fig. 8.

Proof of Theorem 2. The graph G_5 introduced in Remark 1(ii) satisfies the assumptions of Theorem 2; it is embeddable in $\frac{1}{2}\mathbb{H}_{10}$.

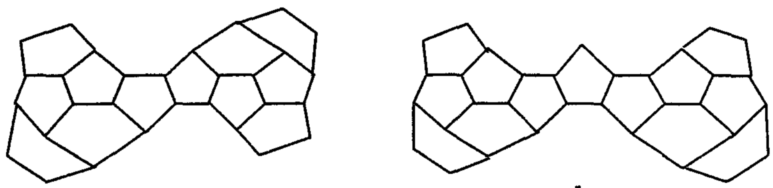
Now suppose $G \neq G_5$, but there is a pentagon in the polypentagon $\Pi(G)$ with 1-neighborhood of the form $\Pi(G_5)$. Then the following seven possibilities for the 2-neighborhood of this pentagon can occur (each of them contains a subgraph from Fig. 8): $\Pi(\mathrm{Do} - v_1 - v_2 - v_3)$, $\Pi(\mathrm{Do} - v_1 - v_2)$, $\Pi(\mathrm{Do} - v - e)$, $\Pi(\mathrm{Do} - e_1 - e_2)$, $\Pi(\mathrm{Do} - v)$, $\Pi(\mathrm{Do} - e)$, $\Pi(\mathrm{Do})$. The last three possible 2-neighborhoods arise only in the three nonserial polypentagons $\Pi(\mathrm{Do} - v)$, $\Pi(\mathrm{Do} - e)$, $\Pi(\mathrm{Do})$; only the polypentagon $\Pi(\mathrm{Do})$ is embeddable. A pentagon with the 1-neighborhood $\Pi(G_5)$ in any other polypenthagon $\Pi(G)$ can have the 2-neighborhood only of one of the other four types. However, all the corresponding 5-graphs are non 5-gonal, and, therefore, they are not embeddable. Let us prove that each of them is isometric. The 2-neighborhood contains not more than three neighbors of the second order. The number of neighbors of the third order can be either one or two. Extending the 2-neighborhood to the 3-neighborhood we easily verify that the edge graph of the 2-neighborhood is an isometric subgraph of the edge graph of the 3-neighborhood. This follows from the fact that some neighbors of the second order of the surrounded pentagon are eliminated and from the simple connectedness of $\Pi(G)$. Moreover, the same argumnet implies that the edge graph of the 2-neighborhood is an isometric subgraph of the whole graph G. Therefore, any graph $G \neq G_5$ satisfying the condition $G_5 \subset G \neq \mathrm{Do}$ is nonembeddable.

Let us show that, under the assumptions of Theorem 2, an alternating zone cannot be closed. Indeed, suppose the converse: a polypentagon $\Pi(G)$ admits a closed alternating edge zone. Then it encloses a subgraph G_3 in $\Pi(G)$ consisting of three pentagons meeting at a common vertex (see Remark 1(ii)). Each of them has a 1-neighborhood of the form $\Pi(G_5)$. Such polypentagon is one of the three, Do $-v$, Do $-e$, or Do, and each of them contains subgraphs from Fig. 8 that do not satisfy the assumptions of Theorem 2.

Now let us show that, under the assumptions of Theorem 2, any cut alternating all edges of a zone in $\Pi(G)$ is convex.

Let k be the number of pentagons of an alternating zone. If $k \geq 5$, then a pentagon adjacent to the zone (if there is one) must be adjacent to one of the extreme pentagons (left or right, since the zone is not closed): otherwise there would be a forbidden subgraph from Fig. 8a (the absence of a forbidden graph from Fig. 8a implies that far from the ends of the zone the boundary of the zone coincides with the boundary of the polycycle $\Pi(G)$; this statement is applicable to both ends). A pentagon adjacent to an end pentagon can occupy one of the three not forbidden positions, where it can be adjacent to three, two, or one pentagon of the zone (in the last case the adjacency is not through an edge, since otherwise we would obtain a zone of length $k+1$).

If $k \geq 6$, then all three possibilities can be realized, and even simultaneously, at each end of the zone: see Fig. 10a for $k = 6$ and Fig. 10b for $k = 7$.



a b

FIG. 10. Zones of length $k = 6$ and $k = 7$ with all possible neighboring pentagons

If k is even, then both banks of a zone have the same length. If there is a pentagon adjacent to the zone through three edges (for k even there is only one such pentagon for each bank of the zone), then substituting the three edges with the other two edges of the pentagon we decrease the length of the polygonal line, which is the boundary between the bank and the adjacent pentagon, by 1. Since closely to the middle of the zone both ends of its boundary belong to the boundary of $\Pi(G)$ and the polypentagon $\Pi(G)$ is simply connected, the ends of a bank of the zone cannot be connected by a shorter path. Therefore, if there is a pentagon adjacent to the zone through three edges, then the distance between the ends of the zone is less than the length of the bank of the zone by one. The argument above implies that, for k even, one of the three following situations can occur:

a) both banks of a zone are geodesic;
b) one of the banks is geodesic, and the other one is not, and the shortest path between the ends of this second bank is shorter than its length and is contained in the corresponding half (determined by the cut);
c) both banks are not geodesic; the shortest distance between the ends of one bank equals the shortest distance between the ends of the second bank (since it is 1 less than the lenght of the bank, and the lengths of the two banks are equal), and each shortest path belongs to its own half (determined by the cut).

In all three cases the cut of the graph under consideration along the edges of the zone is convex.

If k is odd, then one bank of a zone always is geodesic, and its length is 1 less than that of the other bank, which, in its own turn, can be

a) geodesic;
b) not geodesic and such that length of the shortest path between its ends is 1 less than that of the bank, and this path is contained in the corresponding half;
c) not geodesic and such that the length of the shortest path between its ends is 1 or 2 less than that of the bank (the second possibility is realized if there are two pentagons adjacent to the zone through three edges of this bank), and this path is contained in the corresponding half.

In this case the cut is also convex. Indeed, even in case c) if we add two edges to the shortest path between the ends of the bank in order to move the cut into another half, then we obtain a path of length equal to that of the bank. But the length of the second bank (the geodesic one) is 1 less than that of this new path. Hence, it is impossible to move the ends into the other half so as to obtain a smaller distance between them.

We proceed similarly in the cases $1 \le k \le 5$. Here, for example, only one pentagon adjacent to a zone through three edges is allowed because of the prohibition from Fig. 8b. Thus, it is sufficient to study two cases: there is one pentagon adjoining the zone through three edges, or there are no such pentagons. All other adjacencies are admissible, and even simultaneously. In each case the cut along the edges of a zone is convex. For $k = 4$ only one pentagon adjoining the zone through three edges is admissible, and if there is one, then only one of the adjacencies adjoining it is admissible. All other adjacencies are admissible. Similar reasoning works for the remaining cases $k = 3, 2, 1$.

Hence, two zones adjoin each edge of the pentagon. Each cut is convex. We associate with each zone a coordiante axis. As a result, we obtain a mapping of the polypentagon to the hypercube with scale $\lambda = 2$. Theorem 2 is proved. □

Theorem 3. *A simply connected chemical graph without triangles, without quadrangles, and with at most one pentagon is embeddable. In particular, for $r \ge 6$ all poly-r-cycles are embeddable.*

The proof of Theorem 3 is based on the approach of [6], namely, it is easy to verify that all cuts in a graph satisfying the assumptions of Theorem 3 are convex.

Theorem 4. (i) *A mono-3-fusene (one triangle and many hexagons) is embeddable (in $\frac{1}{2}\mathbb{H}_d$, where d is the perimeter) iff the valency of one of the vertices of the triangle is* 2. *In other words, these graphs are embeddable iff they do not contain the isometric subgraph from Fig.* 3a.

(ii) *A di-3-fusene (two triangles and many 6-gons) is embeddable iff each of the two triangles has a vertex of valency* 2.

(iii) *All mono-5-fusenes (fluorenoids) are embeddable (because of Theorem* 3).

(iv) *A mono-4-fusene (biphenylenoid) is embeddable iff it does not contain the isometric subgraph presented in Fig.* 3b.

Proof of Theorem 4. In cases (i), (ii), if there is a triangle with valency of each vertex equal to 3, then this graph contains the forbidden subgraph shown in Fig. 3a, and, therefore, cannot be embeddable. If a triangle has a vertex of valency 2, then, erasing any such triangle, we obtain a subgraph satisfying the assumptions of Theorem 3 and hence embeddable. The recovery of the erased triangle cannot destroy the embeddability.

We emphasize that the two hexagons non incident to the quadrangle (Fig. 3b) are incident to two *opposite* leaves from the vertices of the quadrangle.

In case (iv), if there is a nonconvex zone, then such a zone contains only hexagons, and the shortest path between the two ends of its bank pass through another half of the graph, not adjacent to the given bank. Make the path closed by adding the edges of the bank to it. The path thus obtained encloses the quadrangle. Without loss of generality, we can suppose that the zone touches the quadrangle, since otherwise the bank of the zone would be the shortest path. Hence, the quadrangle adjoins the bank of the zone, and there are two more hexagons adjacent to the quadrangle; this means that we have obtained the forbidden subgraph from Fig. 3b. Theorem 4 is proved. □

Theorem 5. (i) *A di-5-fusene (an indancenoid) is not embeddable if it contains forbidden isometric subgraphs $\Gamma_{s,t}$ depending on two parameters $s, t \in \mathbb{N}$ (see Fig.* 5a) *and corresponding to the values $s = 3$ $t = 2$, subgraphs from Fig.* 5b *corresponding to the values $s = t = 1$, and the forbidden isometric subgraph Γ_u depending on one parameter $u \in \mathbb{N}$. (see Fig.* 5c) *corresponding to the value $u = 3$.*

(ii) *A di-4-fusene (terphenylenoid) is not embeddable if it contains forbidden isometric subgraphs $\Gamma'_{s,t}$ (Fig.* 11a *corresponding to the values $s = 3$ and $t = 2$, Fig.* 11b *corresponding to the values $s = t = 1$), Γ'_u (Fig.* 11c *corresponding to the value $u = 4$, Fig.* 11d *corresponding to the value $u = 1$), and the subgraph shown in Fig.* 3b.

The assumptions of Theorem 5 are obviously necessary since all forbidden graphs from the statement of the theorem are not 5-gonal (five vertices violating the 5-gonal inequality are shown in each figure).

We conjecture that these assumptions are also sufficient for the embeddability of a di-4-fusene (terphenylenoid) and of a di-5-fusene (indancenoid).

Remark 3. It would be interesting to characterize plane fullerenes i.e., partitions of the plane into combinatorial pentagons and hexagons such that the valency of each vertex is three. It is clear that

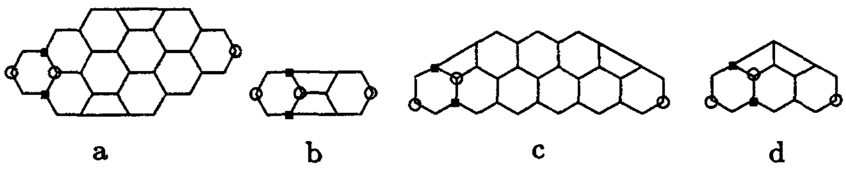


FIG. 11. Forbidden isometric subgraphs of embeddable di-4-fusenes

the number of hexagons in such partition is infinite, and for $p_5 = 0$ or $p_5 = 1$ pentagons there is only one such plane fullerene, while there are infinitely many plane fullerenes with $p_5 = 2$ (see Fig. 5). We are also interested in a description of disk partitions into hexagons and not more than 6 pentagons admitting an extension by hexagons to a partition of the whole plane (with all vertices of valency 3). For example, polypentagons $\Pi(\mathrm{Do})$, $\Pi(\mathrm{Do}-e)$, $\Pi(\mathrm{Do}-v)$, as well as helicenes do not admit such extension. The A. D. Aleksandrov Theorem [15] implies that a plane fullerene with p_5 pentagons exists iff $p_5 \le 6$. Similarly, a partition of the plane into triangles (quadrangles) and hexagons with vertices of valency 3 exists iff $p_3 \le 2$ (resp., $p_4 \le 3$). This follows from the fact that each such partition corresponds to the isometric two-dimensional polyhedron composed of regular Euclidean polygons. The curvature of a polyhedron with this metric is nonnegative (it is strongly positive only in some vertices of the polyhedron). By the Aleksandrov theorem, such polyhedron can be embedded in the 3-space as a convex surface. The total curvature of a convex surface homeomorphic to the plane is not greater than 2π. The contribution of a k-gon in the curvature equals $(6-k)\pi/3$. For a surface consisting of 6- and k-gons, we have $p_k(6-k)\pi/3 \le 2\pi$, i.e., $p_k \le 6/(6-k)$.

Remark 4. (i) Only the following molecular graphs from the list given in [16] are nonembeddable: No.43, Fig. 3.1, NoNo. 43, 44, 46, 48–50, 105–112, 132–136, 168–176, 194–201 (these examples contain a triangle with vertices of valency 3 shown in Fig. 3.2). The handbook [16] does not contain even small forbidden indancenoids presented in Fig. 5. As an example of embeddings of other molecules from [16], note that the *coranulene* $C_{20}H_{10} \to \frac{1}{2}\mathbb{H}_{15}$, the *decacylene* $C_{36}H_{18} \to \frac{1}{2}\mathbb{H}_{33}$; and only *kekulene* $C_{48}H_{24}$ is not 5-gonal.

(ii) A possible direction of research is the study of embeddable graphs C_mH_n in a given class, e.g. indancenoids with $p = (p_5 = 2,\ p_6)$. Examples of synthetic indancenoids are *circofulvalene* (also called semi-buckminsterfullerene) $C_{30}H_{12}$, see Fig. 12a, $C_{30}H_{14}$, $C_{26}H_{12}$. All 45 indancenoids $C_{30}H_{12}$ are presented in [16]. For example, all four indancenoids $C_{15}H_9$ given in [4, Table 1] are embeddable in $\frac{1}{2}\mathbb{H}_{15}$. However, the graph $C_{14}H_8$ given in Fig. 5b is not 5-gonal. And three of the four indancenoids $C_{30}H_{12}$ with the symmetry D_{2h} presented in the same table are not 5-gonal, including the semi-buckminsterfullerene (see Fig. 12a, 12b, 12c). The fourth one, shown in Fig. 12d, is embeddable in $\frac{1}{2}\mathbb{H}_{20}$. Incidentally, the dual graph for the circofulvalene (i.e., the dual graph of the internal faces) is embeddable in $\frac{1}{2}\mathbb{H}_8$.

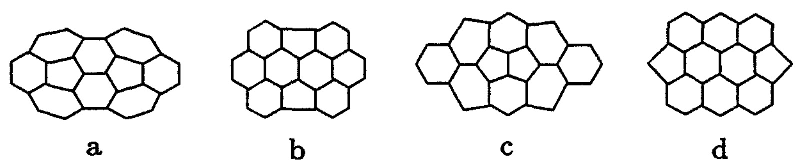


FIG. 12. The four indancenoids $C_{30}H_{12}$ with the symmetry D_{2h}

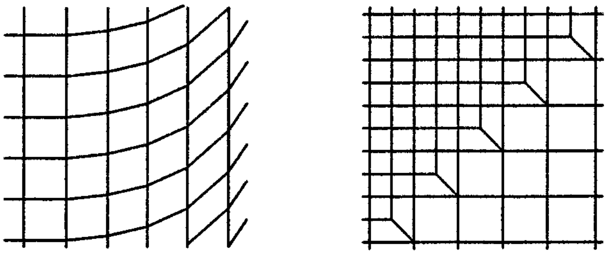
The graphs shown in Fig. 12a and Fig. 12b contain the forbidden isometric subgraph $\Gamma_{2,1}$ from Fig. 5a. The graph shown in Fig. 12c contains the forbidden isometric subgraph $\Gamma_{1,1}$ from Fig. 5b.

(iii) A polyhedron with vertices of valency 3 having $p = (p_5, p_6, p_7)$ $12 + p_7 = p_5$ is called a *fulleroid*. Both minimal icosehedral fulleroids with 260 vertices (see [17]) are not 5-gonal.

Remark 5. A graph G embedded in the plane uniquely determines a closed domain $\Omega(G)$ filled by the internal faces. If $\Omega(G)$ is simply connected and all the internal faces are r-gons such that any two of them either are disjoint, or have a common edge, then the partition of $\Omega(G)$ into the internal faces, which we denoted $\mathbf{II}(G)$, is a poly-r-cycle. This means that precisely three r-gons meet at each vertex of the graph G if this vertex is an internal point of $\Omega(G)$. Now we shall study examples of another kind.

(i) There is a vertex of valency 4. Consider the following mono-q-4-gonal partition of the plane. Attach to each edge of a regular q-gon an infinite chain of squares, and fill in the resulting angles with rhombi. The graph of this partition is embeddable in $\mathbb{Z}_{q/2}$ for q even, and in $\frac{1}{2}\mathbb{Z}_q$ for odd q.

(ii) There are vertices of valency $4, 3, 5$. Figure 13 shows an example of two embeddable infinite poly-4-cycles. One of them (see Fig. 13a) is not a projection of an isometric subgraph from $\mathbb{Z}_d$, $d < \infty$, but this is a zonohedral partition combinatorially equivalent to $\mathbb{Z}_2$. The other one (see Fig. 13b) is embeddable in $\mathbb{Z}_d$ only for $d = \infty$.



a b

FIG. 13. Examples of unusual infinite poly-4-cycles:
a) $\to \mathbb{Z}_2$; b) $\to \mathbb{Z}_\infty$

Remark 6. A *hexagonal torus* (or a *toric benzenoid*) is a normal partition of the torus into hexagons with the valency of each vertex equal to 3. Such tori are studied, for example, in [18]. Denote by T_i such a partition of the torus into i hexagons; clearly, it has $2i$ vertices. T_i is polygonal (i.e., each face is a polygon, and their union is a closed connected 2-manifold) only if $i \geq 7$. The only 7-vertex triangulation of the torus (the Császár torus) has the skeleton K_7 and it is a minimal polyhedron of genus one in $\mathbb{R}^3$ [19].

Examples: benzene-torus $T_3 = K_{3,3}$, the Heawood graph T_7, the pirene-torus T_8, the coronene-torus T_{12}. (T_7 realizes the minimal 7-coloring of the torus.) All of them are not 5-gonal, however the cube γ_3 can be realized as T_4. Incidentally, the edge graphs of all irreducible (in the sense of [20]) quadrangulations of the torus (partitions of the torus into quadrangles) are K_5, $K_6 - 3K_2$, $K_{4,4}$, $K_{3,6}$, $K_{4,5} - P_3$, $K_{5,5} - 5K_2$, $K_7 - C_7$ (see [20]). The first two graphs are embeddable (as the skeletons of α_4 and β_3), and others are not 5-gonal. Two of the ten irreducible quadrangulations of the Klein bottle (see [21]) are embeddable (to be more precise, the skeletons of Q^6 and Q^7 coincide with the emebeddable graphs β_3 and α_3 with pyramids over two faces), and the skeletons of the other eight graphs are not 5-gonal. (The only irreducible quadrangulation of the sphere is C_4, and the projective plane has irreducible quadrangulations K_4 and $K_{3,4}$; only the last of them is nonembeddable.)

Remark 7. The graphs from Remark 6 (as well as the kekulene from Remark 4(i)) provide examples of *not simply connected* poly-6-cycles. Six not simply connected poly-6-cycles are shown in [22, Fig. 2] as examples of possible carbohydrates; all of them are not 5-gonal.

Theorem 6. *There are precisely* 8 *monohedral polypentagons. Three of them are finite*: G_1, G_2, G_3 (*see Remark* 1(ii)), *and the other five are infinite*: *the alternating zone infinite in both directions, the nowhere alternating zone infinite in both directions, the zone with regular interchange of alternation and nonalternation, two nonalternating zones glued together, and the polypentagon from Fig.* 6a.

The proof of Theorem 6 is obtained by exhausting all 1-neighborhoods and complementing them appropriately to monohedral polypentagons. Only in these cases are the 1-neighborhoods of each pentagon in the polypentagon the same. Recall that a polypentagon is called *monohedral* if its symmetry group acts transitively on the r-cycles.

In conclusion, we give an example of a series of embeddable graphs with growing scale having a nonembeddable limit. Take i points A_j on the axes with positive integer coordinate j, $1 \leq j \leq i$. We take two neighboring points A_{j-1} and A_j for a pair of antipodal vertices of the hyperoctahedron β_{n_j} of dimension

$n_j = 2^j$ and add 2^{j-1} new pairs of antipodes (so that only hyperoctahedra with antipodes in adjacent pairs (A_{j-1}, A_j) and (A_j, A_{j+1}) intersect and have the only common vertex A_j). Together, all these hyperoctahedra form the *garland* W_i. The hyperoctahedron β_{n_i}, corresponding to the last pair (A_{i-1}, A_i) is embeddable in $\mathbb{Z}_{m_i}$, where $m_i = 2^i$, with the scale $\lambda_i = 2^{i-1}$. The whole garland W_i is embeddable in the same lattice with the same scale. Denote the limit of W_i as $i \to \infty$ by W_∞. But $\lambda_i \to \infty$ as $i \to \infty$; therefore, there is no embedding of the limit garland W_∞ with a finite scale even in $\mathbb{Z}_\infty$.

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(M. Deza) École Normale Supérieure et CNRS (Paris)
(M. I. Shtogrin) V. A. Steklov Mathematics Institute (Moscow)