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Polyhexes that are ℓ_1 graphs

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ABSTRACT

A connected graph is said to be ℓ_1 if its path distance isometrically embeds into the space ℓ_1. Following the work of Deza, Grishukhin, Shtogrin, and others on polyhedral ℓ_1 graphs, we determine all finite closed polyhexes (trivalent surface graphs with hexagonal faces) that are ℓ_1.

1. Introduction

The path distance on a connected graph Γ is a metric on the set of vertices of Γ. Thus, for each connected graph there is a corresponding metric space. Studying graphs from this point of view is what is sometimes called the *metric graph theory*. One of the advantages of the metric point of view is that it gives a way to define several natural classes of graphs. Indeed, given a collection of "standard" metric spaces, we can define the corresponding class of graphs by requiring that the metric space of the graph should be isomorphic to a subspace of one of the standard spaces. The class of graphs that is central to this paper is defined exactly in this way: A graph Γ is called an ℓ_1 *graph* if and only if the metric space on the vertices of Γ is isomorphic to a subspace of ℓ_1. That is, the vertices of Γ can be matched with some points of ℓ_1 in such a way that the path distance between every two vertices is equal to the distance between the corresponding two points of ℓ_1. We recall that ℓ_1 denotes the set of all real sequences $\{a_n\}$, such that

$$\sum_{i=0}^{\infty} |a_i| < \infty,$$

with distance (metric) on this set defined by

$$d_1(\mathbf{a}, \mathbf{b}) = \sum_{i=0}^{\infty} |a_i - b_i|.$$

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Here, of course, $\mathbf{a} = \{a_n\}$ and $\mathbf{b} = \{b_n\}$ are two points of ℓ_1.

The class of ℓ_1 graphs contains some well-known series of graphs, such as, say, the complete graphs K_n, the cocktail-party graphs $K_{n\times 2}$, the Hamming cubes Q_n, the half-cubes $\frac{1}{2}Q_n$, and some others. Partial cubes, which attracted a lot of attention in recent years (see for example [1–4]), are ℓ_1. The Petersen graph and its complement are both ℓ_1 graphs. The Cartesian product of two ℓ_1 graphs is again ℓ_1. It was noticed early on that the 1-skeleton graphs of the five regular polyhedra are all ℓ_1. This observation motivated the massive search undertaken by Deza, Grishukhin, and Shtogrin, aiming to answer which polytopal graphs (1-skeletons of polytopes) are ℓ_1. The results of that search were summarized in the influential monograph [5].

Among more recent results, we can mention the search for ℓ_1 graphs among the graphs k_n. These are the trivalent plane graphs whose faces are all 6-gons and k-gons (and there is, of course, at least one k-gon). The subscript n refers to the number of vertices of the graph. If $k \geq 6$ then all such graphs are infinite and, furthermore, according to [6] they are all ℓ_1. The picture changes when $k < 6$. First of all, all such graphs are finite. If $k = 3$ then it is easy to see that only the smallest such graph, K_4, is ℓ_1. For $k = 4$, it was shown in [7] that only five of 4_n graphs are ℓ_1. The graphs 5_n are called the fullerene graphs. The name and the motivation to study these graphs come from chemistry. The fullerene graphs that are ℓ_1 were classified in [8]. Again, there are only finitely many (five) such graphs.

In this paper we classify ℓ_1 polyhexes. By a *polyhex* we mean a finite closed polyhex, that is, a finite trivalent surface graph Γ drawn on a surface S in such a way that every face is a hexagon. These graphs are also interesting from the chemistry point of view.

Since Γ is trivalent, every 2-path in Γ lies on a unique face. Furthermore, if two faces share a vertex, they also share a unique edge incident to that vertex. A polyhex is called *polyhedral* if any two faces share a single edge or nothing at all. We view the polyhedral polyhexes as the generic ones, but we do not exclude the nonpolyhedral polyhexes from consideration. In a nonpolyhedral polyhex some two faces share two or three disjoint edges.

Note also that our definition does not exclude loops and multiple edges in Γ. However, as we are interested in ℓ_1 graphs, this point is mute, as neither loops, nor multiple edges are possible in ℓ_1 graphs.

By an easy calculation, the Euler characteristic of the surface S is zero, that is, S is the torus, when S is orientable, or the Klein bottle, when it is nonorientable. We call the corresponding polyhexes *toric* and *Kleinean*.

As the same graph Γ can sometimes be drawn on a surface in several different ways, we will distinguish between the graph Γ and the polyhex Γ. The difference is the polyhex structure, that is, the collection of the face cycles. We will write cycles as closed paths, but we want to make it clear from the start that we view cycles up to the choice of the starting point and/or direction. That is, two closed paths that only differ by the choice of the starting point and/or direction are considered to be the same cycle.

The number N of face cycles is related to the number n of vertices. Indeed, as every 2-path is contained in a unique face cycle, we get $3n = 6N$, that is, $N = \frac{n}{2}$.

We will now state our results. First, we describe the examples of polyhexes that arise in this paper. We start with the infinite series of examples. Let Γ be the n-prism graph, $n \geq 3$. Then we can denote the vertices of Γ as a_i's and b_i's, where the index i is viewed modulo n, in such a way that every a_i is adjacent to a_{i-1}, a_{i+1}, and b_i, and symmetrically, every b_i is adjacent to b_{i-1}, b_{i+1}, and a_i. The n-prism is known to be ℓ_1. Indeed, Γ is the Cartesian product of an edge and an n-cycle, which are both ℓ_1. Let $F_i = a_{i-1}a_ia_{i+1}b_{i+1}b_ib_{i-1}a_{i-1}$. Here i is again understood modulo n, so that we have exactly n hexagons. It is easy to see that every 2-path is contained in a unique hexagon F_i, so the set of F_i provides a valid polyhex structure on Γ. We will denote the resulting polyhex as Γ_{2n}. We leave it to the reader to check that Γ_{2n} is toric for even n and Kleinean for odd n.

Our next example is defined on $\Gamma = K_4$, the complete graph on four vertices. We need $\frac{4}{2} = 2$ face cycles for the polyhex structure. If we denote the vertices as a, b, c, and d, then here is a possible choice of two hexagons: *abcdbca* and *badcadb*. Again, it is easy to see that every 2-path is contained in a unique face cycle, so this is a valid polyhex structure. Note that the face cycles here have self-intersection, but this is allowed by our definition. We denote this example as Γ_4' (leaving the name Γ_4 for the 2-prism, which we disregard because of the multiple edges). The polyhex Γ_4' is Kleinean.

For the next two examples we set $\Gamma = Q_3$, the cube graph. As Q_3 is the same as 4-prism, we have already seen one polyhex structure on this graph. As in the prism example, we denote the vertices of Γ by a_i and b_i, where i is taken modulo four. Let the hexagons F_i be as in the prism example. Note that these hexagons have chords. Namely, F_i contains the chord x_iy_i. The cube Γ also has hexagons that have no chord. Namely, if one removes two opposite vertices of the cube then the remaining six vertices form a hexagon. Let G_i be the hexagon obtained by removing a_i and its opposite, b_{i+2}. For the second polyhex structure we can take F_1, F_3, G_2, and G_4. For the third structure, take all four hexagons G_i. The details that these are valid polyhexes are straightforward. We denote the two new polyhexes by Γ'_8 and Γ''_8, respectively. Looking at the number of face cycles having a chord (four for Γ_8, two for Γ'_8, and zero for Γ''_8) we see that the three polyhexes on the cube graph are pairwise nonisomorphic. We also note that Γ'_8 is Kleinean, while Γ''_8 is again toric, like Γ_8.

In our final example Γ is the 1-skeleton of the cube truncated at two opposite vertices. This polyhedron is sometimes called the Dürer octahedron (or the melancholia octahedron), because it appears in the famous engraving "Melencolia I" by Albrecht Dürer. The graph Γ is known to be ℓ_1, see for example [5], Proposition 5.2. To exhibit the polyhex structure, let us assign names to the vertices of Γ. Recall that the cube graph with two opposite vertices removed is a hexagon. We can denote these six vertices as a_i, where i is taken modulo six, and each a_i is adjacent to a_{i-1} and a_{i+1}. One of the removed vertices was adjacent to the vertices a_i with i even, while the second removed vertex was adjacent to a_i's with i odd. So in Γ, in addition to a_i's, we have vertices b_i, where i is again taken modulo six, and every b_i is adjacent to a_i, b_{i-2}, and b_{i+2}. The polyhex structure consists of the six hexagons $F_i = a_ia_{i+1}b_{i+1}b_{i+3}b_{i-1}a_{i-1}a_i$. This polyhex is Kleinean; it will be denoted by Γ'_{12}.

Here is our main theorem.

Theorem 1.1. *If Γ is an ℓ_1 polyhex then either Γ is the prism polyhex Γ_{2n}, $n \geq 3$, or one of the four sporadic examples Γ'_4, Γ'_8, Γ''_8, or Γ'_{12}.*

To prove this result we utilize the labels on ℓ_1 graphs. This technique originated from [9,10]. It was also used in [7,8]. In Section 2 we briefly review the basics of labels. In Sections 3 and 4 we present the proof of Theorem 1.1. Namely, in Section 3 we classify all ℓ_1 polyhexes, where some face cycle is not isometric. These are considered as "small", or "exceptional" polyhexes. After that, in Section 4 we do the "generic" case, where all faces are isometric. Although the generic case contains most of the polyhexes, under the ℓ_1 condition it only brings one example, Γ''_8.

2. Labels on ℓ_1 graphs

Recall that the Hamming cube graph Q_n can be realized as follows. Let $\Omega = \{1, 2, \ldots, n\}$. We will call the elements of Ω the *coordinates* of Q_n. The vertices of Q_n are all subsets of Ω. Two subsets A and B are adjacent if and only if they differ in a single element, that is, if $|A \triangle B| = 1$. Here $\triangle$ denotes the symmetric difference of sets, *i.e.*, $A \triangle B = (A \setminus B) \cup (B \setminus A)$. In general, the distance in Q_n between two subsets A and B of Ω equals $|A \triangle B|$.

A mapping ϕ from Γ to Q_n is a scale λ embedding if $d_{Q_n}(\phi(u), \phi(v)) = \lambda d_\Gamma(u, v)$ for all vertices u and v of Γ. Assouad and Deza showed in [11] that a finite graph is ℓ_1 if and only if it has a scale λ embedding in Q_n for some λ and n.

Let Γ be a finite ℓ_1 graph and ϕ be a scale λ embedding of Γ in Q_n. Using ϕ we assign to each edge uv a *label* $\ell(uv)$ as follows: $\ell(uv) = \phi(u) \triangle \phi(v)$. Every label consists of exactly λ coordinates. We will need the following properties of labels. The proofs can be found in, say, [10], see Lemma 4.2 there.

Lemma 2.1. *If $\gamma = uu_1u_2 \ldots u_{k-1}v$ is a path from u to v then $\phi(u) \triangle \phi(v) = \ell(uu_1) \triangle \ell(u_1u_2) \triangle \ldots \triangle \ell(u_{k-1}v)$. Furthermore, if γ is geodesic, that is, if $d_\Gamma(u, v) = k$, then the labels $\ell(uu_1)$, $\ell(u_1u_2), \ldots, \ell(u_{k-1}v)$ are pairwise disjoint and $\phi(u) \triangle \phi(v) = \ell(uu_1) \cup \ell(u_1u_2) \cup \cdots \cup \ell(u_{k-1}v)$. In particular, every edge label on every shortest path from u to v is contained in $\phi(u) \triangle \phi(v)$.* $\square$

Recall that a subgraph of Γ is *isometric* if the distance in the subgraph between any two vertices equals the distance in Γ between the same two vertices. For two edges in a k-cycle graph we say that they are *opposite* if they are at the maximum possible distance. Thus, if k is even then every edge has a unique opposite edge, while if k is odd then every edge has two opposite edges.

Lemma 2.2. *Suppose that Δ is an isometric subgraph of Γ isomorphic to the k-cycle. Suppose further that uv and wz are opposite edges of Δ. If k is even then $\ell(uv) = \ell(wz)$, while if k is odd then $|\ell(uv) \cap \ell(wz)| = \frac{\lambda}{2}$ (in particular, λ must be even).* □

Notice that Lemma 2.1 implies that if uv and wz are not opposite then $\ell(uv)$ and $\ell(wz)$ are disjoint, unless of course the two edges coincide. Also, it follows that if k is odd and, say, zt is the second edge opposite to uv then $\ell(uv) \subset \ell(wz) \cup \ell(zt)$.

From this point on, Γ is an ℓ_1 polyhex. We fix a scale embedding of Γ into a suitable Hamming cube and assign labels to the edges, as described above.

3. Nonisometric faces

In this section we deal with all the cases where at least one face cycle C is not isometric. First, we consider the case where C has a self-intersection. Since Γ has no double edges, two vertices of C can coincide only if they are at distance three in C.

Lemma 3.1. *If Γ has a face cycle with a self-intersection then Γ is the polyhex Γ_4'.*

Proof. Suppose that $C = abcdefa$ is the face cycle having self-intersection. By the comment before the lemma, we can assume that, say, $a = d$. As Γ has valency three, b, c, e, and f cannot be all distinct. So $b = e$, or $c = f$. Without loss of generality, assume that $b = e$. If also $c = f$ then C passes twice through cab; clearly, a contradiction. So $c \neq f$.

First suppose that c and f are not adjacent. Let g be the third neighbour of c, and h the third neighbour of f. Then $gcafh$ and $gcbfh$ are parts of two different face cycles, say, $C_1 = gcafhxg$ and $C_2 = gcbfhyg$. Note that in particular $g \neq h$, as they are at distance two in C_1 (and C_2). Also, $x \neq y$, since C_1 and C_2 cannot share a 2-path. Among the vertices above, only x and y have free valencies. This implies that both C_1 and C_2 are isometric. Let us take a look at the labels. Since C_1 is isometric, $\ell(af) = \ell(gx)$ by Lemma 2.2. Also, $\ell(af) \subset \ell(bf) \cup \ell(bc)$, and since $\ell(af) \neq \ell(bf)$, we must have $\ell(af) \cap \ell(bc) \neq \emptyset$. Hence $\ell(gx) \cap \ell(bc) \neq \emptyset$, which means that $d_\Gamma(x, b) < 3$. However, the neighbours of b are a, c, and f. Clearly, x is neither equal, nor adjacent to either of these vertices; a contradiction.

Thus, c and f are adjacent. As all four vertices have no free valencies and Γ is connected, we conclude that $\Gamma \cong K_4$. Finally, it is now easy to see that our polyhex has exactly two faces, C and $C' = cafcbfa$. So the polyhex structure is unique, and $\Gamma = \Gamma_4'$. □

From now on we assume that no face cycle of Γ has a self-intersection.

Lemma 3.2. *Any two 3-cycles in Γ are disjoint.*

Proof. Suppose to the contrary that Γ contains two 3-cycles, $abca$ and $adea$, sharing the vertex a. Since Γ has valency three, the vertices b, c, d, and e cannot be all distinct. Without loss of generality, assume that $b = d$. Now let C be the face cycle passing through acb. Since C has no self-intersection, a cannot follow b on C, so e must follow b, as c, a, and e are the only neighbours of b. Similarly, e must precede a on C. This is a contradiction, as C passes through e twice. □

Corollary 3.3. *If $C = abcda$ is a 4-cycle with $a \neq c$ and $b \neq d$ then C is isometric.*

Proof. If a is adjacent to c, or b is adjacent to d then two 3-cycles sharing a common edge arise, contrary to Lemma 3.2. □

We next deal with the cases where the nonisometric face cycle contains a *chord*, *i.e.*, an edge between nonconsecutive vertices of the cycle. The distance in the face cycle between the ends of the chord is either two, or three. We call such chords *short*, or *long*, respectively.

Lemma 3.4. *No face has two long chords.*

Proof. By contradiction, suppose that $C = abcdefa$ is a face cycle with two long chords; say, a is adjacent to d, and b is adjacent to e. By Corollary 3.3, the 4-cycle $abeda$ is isometric. So Lemma 2.2 yields that $\ell(ab) = \ell(de)$. Similarly, $abefa$ is isometric, and so $\ell(ab) = \ell(ef)$. Hence $\ell(de) = \ell(ef)$, implying that $d = f$, a contradiction. □

Lemma 3.5. *Suppose a face cycle C has two chords. Then Γ is the* 3*-prism polyhex Γ_6.*

Proof. By Lemma 3.4, at least one of the chords is short. So, without loss of generality, $C = abcdefa$ and a is adjacent to c. Since Γ has valency three, a second chord cannot start at a or c. Furthermore, by Lemma 3.2, the second chord cannot connect b with d, and similarly, it cannot connect b with f. So the second chord either connects b with e, or it connects d with f.

Suppose that b is adjacent to e. Let us take a look at the labels. First of all, $\ell(ab) \cap \ell(bc) \neq \emptyset$, since a and c are adjacent. Also, the 4-cycles $bcdeb$ and $bafeb$ are isometric. Hence, by Lemma 2.2, $\ell(ab) = \ell(ef)$ and $\ell(bc) = \ell(de)$. So $\ell(de) \cap \ell(ef) \neq \emptyset$, which implies that d and f are adjacent. This means that Γ is the 3-prism, as claimed.

Suppose now that d is adjacent to f. Let D be the face cycle passing through acd. Since D and C cannot share a 2-path, f must follow d on D. Since D cannot have a self-intersection, e must follow f. Similarly, b must precede a. Now it is clear that $D = bacdfeb$, that is, b and e must be adjacent, and we are back to the 3-prism.

The polyhex structure on Γ is unique. Indeed, the 3-prism has exactly three 6-cycles having no self-intersections, and by counting all three must be face cycles. So $\Gamma \cong \Gamma_6$. □

Lemma 3.6. *Suppose a face cycle C contains a single chord, which is short. Then $\Gamma \cong \Gamma'_{12}$.*

Proof. Suppose that $C = abcdefa$, and the short chord connects a and c, that is, a and c are adjacent. If Γ has a face with two chords then by Lemma 3.5 Γ is the 3-prism. However, in this case every face has two chords, a contradiction. Hence every face of Γ has at most one chord.

Let g be the third neighbour of b. Let D and E be the face cycles passing through bca and cab, respectively. Then $D = bcafhgb$ and $E = cabgkdc$ for some vertices h and k. We note that the vertices a, b, c, d, e, f, g, h, and k are pairwise distinct. Indeed, the first six vertices are on C, which has no self-intersection. Furthermore, since C has only one chord, g, h, and k are not on C. It remains to see that g, h and k are pairwise distinct. The vertices g and h belong to D and hence they are distinct. Similarly, g and k are distinct since they are together on E. Finally, if $h = k$ then D and E share a 2-path bgh; a contradiction. Within our configuration of nine vertices, only e, h, and k have unused valencies. We next claim that no two of these three vertices are adjacent. Indeed, suppose, say, e and h are adjacent. Then the face cycle F passing through efh cannot continue to g, since it cannot share a 2-path with D. Hence F should continue to e, which makes F self-intersect; a contradiction.

Let l, m, and n be the third neighbours of e, h, and k, respectively. Then $lefhm$, $mhgkn$, and $nkdel$ are contained in three face cycles F, G, and H, respectively. In particular, this means that the three new vertices are pairwise distinct.

Let $F = lefhmol$, $G = mhgknpm$, and $H = nkdelqn$ for some vertices o, p, and q. If one of these faces, say F, has a chord then the chord in F can only be between l and m. Then $m = q$ and $l = p$, and so we also must have $n = o$. This completes the graph Γ, which turns out to be the cube with two opposite vertices truncated, as in Γ'_{12}.

Thus, we can now assume that neither of the face cycles F, G, and H has chords. Since on F only o has unused valencies, we conclude that F is isometric, and similarly, G and H are also isometric. By observation, also the 6-cycle $efhgkde$ is isometric. Let us look at the labels. By Lemma 2.2, $\ell(de) = \ell(gh)$. Also, $\ell(de) = \ell(nq)$ and $\ell(gh) = \ell(np)$. So $\ell(nq) = \ell(np)$, implying $p = q$. However, this means that G and H share the 2-path knp, a contradiction.

So Γ is indeed the cube with two opposite vertices truncated. Let us see that the structure of the polyhex is unique. Counting yields that there must be six faces. The graph contains six 6-cycles having a chord, and one 6-cycle ($efhgkde$, above) having no chord. The latter cycle meets all other 6-cycles in a 2-path, so it cannot be a face cycle. So the six 6-cycles with chords must be the face cycles, and Γ is the polyhex Γ'_{12}. □

Corollary 3.7. *If Γ contains a* 3*-cycle then it is one of the polyhexes above.* □

We now assume that Γ contains no 3*-cycles.* In particular, only long chords are possible.

Lemma 3.8. *Suppose that $C = abcdefa$ is a face with the long chord ad. If $bade$ is part of a face cycle then Γ is the polyhex Γ_8'.*

Proof. Let D be the face containing $bade$, say, $D = badexyb$ for some vertices x and y. Clearly, $x \neq f$, so x is the third neighbour of e (the one that is not adjacent to e in C), and similarly, y is the third neighbour of b.

If x is on C then ex is a chord of C and so, by assumption, we must have that $x = b$, which is impossible since Γ has no multiple edges. Thus, x is not on C and, similarly, y is not on C, either.

We claim that D is isometric. First of all, as only x and y can have new neighbours, D has no chords. It remains to see that vertices that are at distance three in D cannot be at distance two in Γ. Clearly, b and e cannot be at distance two. If a and x are at distance two then x must be adjacent to f, leading to a 3-cycle. Similarly, if d and y are at distance two then y must be adjacent to c, again leading to a 3-cycle.

Thus, D is isometric, which according to Lemma 2.2 means that $\ell(ad) = \ell(xy)$. By Corollary 3.3, the 4-cycle $adefa$ is isometric. Applying again Lemma 2.2, we get $\ell(ad) = \ell(ef)$. Hence $\ell(ef) = \ell(xy)$, which yields that f and y are adjacent. Similarly, from the 4-cycle $adcba$ we get $\ell(ad) = \ell(bc)$. This gives $\ell(bc) = \ell(xy)$, and hence c is adjacent to x. We conclude that the graph Γ is the cube. The complete polyhex structure is easy to recover. In addition to C and D, we must also have face cycles $E = fadcxyf$ and $F = acbyfea$. So Γ is the polyhex Γ_8'. □

We now additionally assume that Γ is not as in Lemma 3.8. This means that if $C = abcdefa$ is a face with a long chord ab then there exist face cycles D and E containing $badc$ and $fade$, respectively. We call D and E the *neighbours* of C. Manifestly, D and E have long chords and, furthermore, C is a neighbour of both D and E. So we get a graph Δ on the set of faces with chords, where every such face is adjacent to two further faces. Since Γ is finite, every connected component of Δ is a cycle. Let $C_0 = C, C_1, \ldots, C_n$ be the faces in the connected component containing C. We will let the index i run through the entire $\mathbb{Z}$ in such a way that $C_i = C_{i+n}$ for all i. We also assume that C_{i-1} and C_{i+1} are the neighbours of C_i for all i.

Lemma 3.9. *Suppose a face cycle C has a long chord. Then Γ is the n-prism polyhex Γ_{2n}, for $n \geq 4$.*

Proof. We adopt the notation introduced before this lemma. We will also need notation for the vertices involved in the cycles C_i. We let $C_i = x_i x_{i+1} x_{i+2} y_{i+2} y_{i+1} y_i x_i$, where $x_0 = f$, $x_1 = a$, $x_2 = b$, $y_0 = e$, $y_1 = d$, and $y_2 = c$. Set $L = \ell(ab)$. By Corollary 3.3, all 4-cycles $x_i x_{i+1} y_{i+1} y_i x_i$ are isometric. Using Lemma 2.2 repeatedly, we see that $\ell(x_i y_i) = L$ for all i.

Clearly, the edge $x_i y_i$ coincides with $x_{i+n} y_{i+n}$ for all i. We claim that, furthermore, $x_i = x_{i+n}$ and $y_i = y_{i+n}$. By contradiction, suppose $x_i = y_{i+n}$ and $y_i = x_{i+n}$. Then $x_i x_{i+1} \ldots x_{i+n}$ is a path connecting x_i with $y_i = x_{i+n}$. By Lemma 2.1, the label $\ell(x_i y_i) = L$ is the symmetric difference of all the labels $\ell(x_j x_{j+1})$ along the above path. Hence there must be a label $\ell(x_j x_{j+1})$ that is not disjoint from L. This leads to a contradiction since $\ell(x_j y_j) = L$ and the 4-cycle $x_j x_{j+1} y_{j+1} y_j x_j$ is isometric. Thus $x_i = x_{i+n}$ and $y_i = y_{i+n}$ for all i.

If $x_i = x_j$ or y_j with $i \not\equiv j \bmod n$ then, because of the labels, $x_i y_j = x_j y_j$. Since Γ has valency three, C_i and C_j must share $x_{i-1} x_i x_{i+1}$, which means that $C_i = C_j$, a contradiction. So we have constructed a configuration consisting of exactly $2n$ vertices. Furthermore, each vertex has the full valency three within the configuration. Since Γ is connected, we conclude that Γ is indeed the n-prism. Since Γ contains no 3-cycles, we have $n \geq 4$.

Manifestly, the polyhex structure consists of all cycles C_i. □

So far we classified all ℓ_1 polyhexes having a face with a self-intersection or with a chord. The following lemma now makes a bridge to the generic case.

Lemma 3.10. *Suppose that no face cycle in Γ has a chord. Then all face cycles are isometric.*

Proof. By contradiction, suppose that the face $C = abcdefa$ is not isometric. Then, by assumption, two opposite vertices on C must have distance two in Γ. Say, a and d have a common neighbour x. Since C has no chords, x does not lie on C. Let D be the face cycle containing axd. By symmetry, we can assume that D continues to e after d. Which vertex precedes a? It must be either b or f. If it is f then D has a chord fe, a contradiction. So $D = baxdeyb$ for some vertex y, a joint neighbour of b and e. Thus b and e are at distance two in Γ.

We claim that c and f also are at distance two from each other. For this let us take a look at the labels. Note that, since Γ contains no 3-cycles, every 5-cycle in Γ is isometric. Looking at the 5-cycle $abyefa$, we see by Lemma 2.2 that $\ell(ef)$ is contained in $\ell(by) \cup \ell(ab)$. Since the edge bc is adjacent to both by and ab, we have that $\ell(bc)$ is disjoint from both $\ell(by)$ and $\ell(ab)$. Hence $\ell(bc) \cap \ell(ef) = \emptyset$. Next we look at the 5-cycle $bcdeyb$. Since bc and de are opposite in this cycle, by Lemma 2.2 we have that $T = \ell(bc) \cap \ell(de)$ has size $\frac{1}{2}|\ell(bc)|$. Finally, let us focus on the 5-cycle $axdefa$. Here de is opposite to af and ef. So by Lemma 2.2 we must have that $\ell(de) \subset \ell(af) \cup \ell(ef)$. Now recall that $\ell(bc)$ and $\ell(ef)$ are disjoint. This implies that $T \subset \ell(af)$. Therefore, the labels of the edges bc and af are not disjoint, which yields that c and f cannot be at distance three from each other.

Since C has no chords, c and f must be distance two apart. Now we are prepared for the final contradiction. Let z be the common neighbour of c and f and let E be the face cycle passing through czf. By symmetry we can assume that E continues to a after f. Since E cannot have a chord, d must precede c on E. It is now clear that $E = dczfaxd$, since x is the only common neighbour of a and d. We conclude that E and D share axd, which is a contradiction. □

To summarize, in this section we have proven that if the polyhex Γ has a nonisometric face then it is either the prism polyhex Γ_{2n}, or one of the three additional examples, Γ'_4, Γ'_8, and Γ'_{12}. In the next section we take on the generic case of polyhexes with isometric faces. There we will encounter the last example of ℓ_1 polyhexes.

4. Isometric faces

Throughout this section we assume that Γ is a polyhex, in which all faces are isometric. Combining this with the ℓ_1 condition, we get the following.

Lemma 4.1. *Opposite edges on a face carry the same label.* □

Before we deal with the general case, let us consider the particular case where the last example of an ℓ_1 polyhex arises.

Lemma 4.2. *Suppose that Γ contains a 4-cycle. Then Γ is the polyhex Γ''_8.*

Proof. Suppose that $abcda$ is a 4-cycle. Let C be the face passing through abc. Then $C = abcxyza$ for some vertices x, y, and z. Since faces of Γ have no chords, $x \neq d \neq z$. Also, let D be the face cycle passing through cda. Then $D = cdazuxc$ and $u \neq y$. Let us look at the labels. Since Γ contains no 3-cycles, every 4-cycle is isometric. Hence $\ell(ab) = \ell(cd)$. Since D is isometric, we get $\ell(cd) = \ell(zu)$. Thus, $\ell(ab) = \ell(zu)$. Combining labels along $bazu$, we see that two equal labels cancel, and so b and u must be adjacent. Similarly, we show that d and y are adjacent, which means that Γ is the cube.

The cube has exactly four isometric 6-cycles, and so all of them must be faces. □

From now on we assume that Γ has no 4-cycles. There are no further examples left, and so we will aim now to arrive at a contradiction in all remaining subcases.

We next introduce zigzags and railroads, discuss the relationship between them, and get some important consequences on the way.

Let $\gamma = \dots x_{-1}x_0x_1x_2\dots$ be a path infinite in both directions. We also assume that γ has no returns, that is, $x_i \neq x_{i+2}$ for all i. Let F_i be the face passing through $x_{i-1}x_ix_{i+1}$. Then we say that γ is a *zigzag* if $F_i \neq F_{i+1}$ for all i. The face F_i will be called the *side face* of γ at x_i. If we select an orientation at one vertex x_i and then carry it along γ then a left turn on γ is followed by a right turn and vice versa. This explains the name "zigzag". We take with zigzags the same approach as with cycles. Namely, two zigzags differing from each other only by a shift of indices and/or change of direction are considered to be the same.

Note that if we know three consecutive vertices of a zigzag then the continuation is unique in both direction. Hence every 2-path, that is not a return, is contained in a unique zigzag. In particular, if $x_{i-1}x_ix_{i+1}$ coincides with $x_{j-1}x_jx_{j-1}$ then $x_k = x_{k+n}$ for all k, where $n = i - j$. Since Γ is finite, it contains a finite number of different 2-paths, and so there must exist $n > 0$ such that $x_i = x_{i+n}$ for all i. The smallest n like that is called the *length* of the zigzag. Associated with γ, there is a cycle $x_0x_1 \dots x_n$, which we will call the *zigzag cycle*, or simply zigzag, where no confusion may result. Recall that we view cycles up to the choice of direction and the origin. In particular, $x_ix_{i+1} \dots x_{i+n}$ is the same cycle, no matter which i we choose.

For a zigzag γ, let y_i be the third neighbour of x_i (*i.e.*, the neighbour not equal to x_{i-1} or x_{i+1}). The edge $e_i = x_iy_i$ will be called the *side edge* to γ at x_i, and the label $\ell(e_i)$ will be called the *side label*.

Lemma 4.3. *Suppose that γ is a zigzag. Then e_{i-1} and e_{i+1} are opposite edges of F_i. In particular, $\ell(e_{i-1}) = \ell(e_{i+1})$. Furthermore, $\ell(e_i) \neq \ell(e_{i+1})$.*

Proof. Since $F_i \neq F_{i+1}$, x_{i+2} does not follow x_{i+1} on F_i. Similarly, x_{i-2} does not precede x_{i-1} on F_i. Since Γ is trivalent, $F_i = x_ix_{i+1}y_{i+1}zy_{i-1}x_{i-1}x_i$ for some vertex z. Manifestly, e_{i-1} and e_{i+1} are opposite to each other on F_i. So they must carry the same label, since F_i is isometric.

Suppose $\ell(e_i) = \ell(e_{i+1})$. Then, combining the labels along $y_ix_ix_{i+1}y_{i+1}$, we determine that y_i and y_{i+1} are adjacent; a contradiction, since Γ contains no 4-cycles. □

Using this lemma and induction, we establish the following.

Corollary 4.4. *Side labels at x_i and x_j are equal if and only if $i \equiv j$ mod 2.* □

Now the following key fact follows.

Corollary 4.5. *All zigzags have even length.* □

Proof. If γ is a zigzag of length n and e_i's are the side edges then $e_n = e_0$ and so, obviously, e_n and e_0 carry the same label. By Corollary 4.4, $n = n - 0$ is even. □

Given two cycles C and D having a common subpath T, we may combine the complements of T in C and D to form a new cycle, which we call the *product* of C and D. We note that in general the product of C and D is not uniquely defined, so this is not a proper algebraic operation, and the term "product" simply refers to the way in which the new cycle is obtained. We also note that this construction can be used repeatedly, and so we can talk of products of three and more cycles.

Corollary 4.5 works best in conjunction with the following.

Lemma 4.6. *Every cycle in Γ is a product of faces and zigzag cycles.*

Proof. By contradiction, suppose that $\gamma = x_0x_1 \dots x_{k-1}x_0$ is the shortest cycle that is not a product of faces and zigzags. If γ is not isometric then it is a product of two shorter cycles, which leads to a contradiction. Thus, γ is isometric. For every $i \in \mathbb{Z}$, set $x_i = x_r$, where r is the remainder of i divided into k. Also, let F_i be the face cycle passing through $x_{i-1}x_ix_{i+1}$. Since γ cannot be a zigzag cycle, for some i we must have $F_i = F_{i+1}$. This means that $F_i = x_{i-1}x_ix_{i+1}x_{i+2}uwx_{i-1}$ for some vertices u and w. Construct γ' from γ by substituting the subpath $x_{i-1}x_ix_{i+1}x_{i+2}$ with $x_{i-1}wux_{i+2}$. Note that, since γ is isometric, u and w are not on γ, and hence γ' is a cycle of the same length as γ. Manifestly, γ is the product of γ' and the face F_i, so γ' in turn cannot be a product of faces and zigzags. In particular, γ' is also isometric.

Let e be the edge of γ that is opposite to $x_{i-1}x_i$, but not to x_ix_{i+1}. Then e also lies on γ'. Moreover, in γ' the edge e is opposite to $x_{i-1}w$, but not to wu, and hence also not to ux_{i+2}. However, $x_{n-1}x_i$ and ux_{i+2} are opposite edges of F_i, and so they carry the same label by Lemma 2.2. This leads to a contradiction, since the labels of e and of ux_{i+2} must be disjoint, while the labels of e and $x_{n-1}x_i$ are equal or share half of their coordinates. □

We now derive some important consequences of Corollary 4.5 and Lemma 4.6.

Corollary 4.7. *The graph Γ is bipartite. In particular, every label consists of a single coordinate.*

Proof. By Corollary 4.5 all zigzags have even length. Also, all faces manifestly have even length. A product of two cycles of even length again has an even length. It now follows from Lemma 4.6 that all cycles in Γ have even length. Hence Γ is bipartite. The last claim follows from [9]. $\square$

Another significant simplification of the picture comes from the following.

Lemma 4.8. *Face and zigzag cycles preserve orientation.*

Proof. Face cycles are boundaries of disks, so they clearly preserve orientation.

Consider a zigzag γ of length $n = 2k$. Pick an orientation $O = O_0$ at x_0 and carry it along γ to an orientation O_1 at x_1, orientation O_2 at x_2, and so on. Eventually we arrive at $x_n = x_0$ with an orientation $O' = O_n$. We need to show that $O = O'$.

We have already mentioned that the turns alternate on a zigzag. That is, if, say, γ makes a left turn at x_0 with respect to $O = O_0$ then it makes a right turn at x_1 with respect to O_1, and so on. That is, γ makes a left turn with respect to O_i at every x_i with i even, and a right turn at every x_i with i odd. In particular, since n is even, γ makes a left turn at $x_n = x_0$ with respect to $O' = O_n$. Since it also makes a left turn with respect to O, we must have $O' = O$. $\square$

Corollary 4.9. *The surface S is orientable, that is, S is a torus.*

Proof. The surface S is orientable if and only if every cycle on Γ preserves orientation. If two cycles preserve orientation then their product also preserves orientation. So the claim follows from Lemmas 4.6 and 4.8. $\square$

Before we turn to railroads, we prove some further properties of zigzags.

Lemma 4.10. *Suppose that $\gamma = \dots x_{-1}x_0x_1x_2\dots$ is a zigzag of length n. Then $x_i = x_j$ if and only if $i \equiv j \bmod n$.*

Proof. By contradiction, suppose that $x_i = x_j$, where $k = j - i > 0$ is minimal subject to $i \not\equiv j \bmod n$. Clearly, $k < n$.

First assume that k is odd. Then the side edges x_iy_i at x_i and $x_{j+1}y_{j+1}$ at x_{j+1} carry the same label by Corollary 4.4. Looking at the 3-path $y_ix_ix_{i+1}y_{j+1}$ we conclude that y_i and y_{j+1} are adjacent, which leads to a 4-cycle, a contradiction. Hence k is even.

Since the side edges at x_i and x_j carry the same label, they must in fact coincide. Hence $\{x_{i-1}, x_{i+1}\} = \{x_{j-1}, x_{j+1}\}$. In view of the minimality of k, we must have further that $x_{i-1} = x_{j-1}$ and $x_{i+1} = x_{j+1}$. Iterating this argument in both directions along γ, we establish that $x_s = x_{s+k}$ for all s; a contradiction, since $0 < k < n$. $\square$

Corollary 4.11. *Zigzag cycles have no self-intersections.* $\square$

We strengthen this as follows.

Lemma 4.12. *Zigzag cycles are isometric.*

Proof. Suppose that $\gamma = \dots x_{-1}x_0x_1x_2\dots$ is a zigzag of length n and $C = x_0x_1\dots x_n$ is the corresponding cycle. Suppose that C is not isometric and choose two vertices, a and b, of C such that the distance between a and b in Γ is smaller than the distance between them in C. We may assume that the distance in C between a and b is smallest among all such pairs. Let $ac\dots b$ be the shortest path in Γ between a and b. By the minimality, c does not lie on C, that is ac is a side edge at a, and so $L = \ell(ac)$ is a side label. Since a and b can also be connected by a path in C, we conclude that one of the labels $\ell(x_ix_{i+1})$ equals L. (Recall that every label consists of a single coordinate.) This leads to a contradiction. Indeed, L equals the side label at x_i or at x_{i+1} by Corollary 4.4, and so L cannot be equal to $\ell(x_ix_{i+1})$. $\square$

Note that this argument in fact shows that every zigzag cycle is convex. We now turn to the next concept.

A *railroad* is a sequence of edges $T = \dots t_{-1}t_0t_1t_2\dots$, infinite in both directions, such that t_i and t_{i+1} are opposite edges of some face T_i, for all i. We note that T_i is uniquely determined by this condition, since Γ has no 4-cycles and no 5-cycles. We call the T_i's the *connecting faces* of T. As with the cycles and zigzags, we will view two railroads obtained from each other by a shift of indices and/or reversal of the direction as being the same. With this understanding, every edge is contained in a unique railroad. The *length* of the railroad T is the smallest positive n such that $t_i = t_{i+n}$ for all i.

The following property follows directly from Lemma 4.1.

Lemma 4.13. *All edges of a railroad carry the same label.* $\square$

Thus, we can speak of the labels carried by railroads.

Let us now discuss the relation between zigzags and railroads. First, suppose that $\gamma = \dots x_{-1}x_0x_1x_2\dots$ is a zigzag with side edges x_iy_i. Let t_j be the side edge $x_{2j}y_{2j}$ and s_j be the side edge $x_{2j+1}y_{2j+1}$. Then it follows from Lemma 4.3 that $T = \dots t_{-1}t_0t_1t_2\dots$ and $S = \dots s_{-1}s_0s_1s_2\dots$ are two railroads. Furthermore, Corollary 4.4 tells us that T and S carry different labels, therefore $T \neq S$. We call these T and S the *side railroads* of γ.

Conversely, suppose that $T = \dots t_{-1}t_0t_1t_2\dots$ is a railroad with connecting faces T_i. Suppose $t_i = u_iv_i$, where we can assume that u_i and u_{i+1} are at distance two for all i, that is, they have a common neighbour w_i. Note that v_i and v_{i+1} then also must be at distance two from each other. Let z_i be the common neighbour of v_i and v_{i+1}. With this notation we have $T_i = u_iw_iu_{i+1}v_{i+1}z_iv_iu_i$. From this it follows that T_i is not equal to the face containing $w_{i-1}uw_i$, and similarly, T_i is not equal to the face containing $w_iu_{i+1}w_{i+1}$. This means that $\gamma = \dots w_{-1}u_0w_0u_1\dots$ is a zigzag. Similarly, $\rho = \dots z_{-1}v_0z_0v_1\dots$ is a zigzag. We will call γ and ρ the *boundary zigzags* of T. Note that Lemma 4.12 implies that $\gamma \neq \rho$.

Lemma 4.14. *If γ is a zigzag of length n then its side railroads have length $k = \frac{n}{2}$. Conversely, if T is a railroad of some length k then its boundary zigzags have length $n = 2k$.*

Proof. Let $\gamma = \dots x_{-1}x_0x_1x_2\dots$ be a zigzag with side edges x_iy_i and let $T = \dots t_{-1}t_0t_1t_2\dots$, where $t_j = x_{2j}y_{2j}$. Clearly, $t_j = t_{j+k}$, where $k = \frac{n}{2}$. Suppose $t_j = t_m$ with $0 < |j - m| < k$. This gives us $\{x_{2j}, y_{2j}\} = \{x_{2m}, y_{2m}\}$. Furthermore, if $x_{2j} = y_{2m}$ then γ must coincide with the other boundary zigzag of T, which is impossible. Hence, $x_{2j} = x_{2m}$, which leads to a contradiction with Lemma 4.10.

Conversely, suppose $T = \dots t_{-1}t_0t_1t_2\dots$ be a railroad of length k and let T_i, u_i, v_i, w_i, and z_i be as above. Let $\gamma = \dots w_{-1}u_0w_0u_1\dots$. Set $x_{2j} = u_j$ and $x_{2j-1} = w_j$ for all j, so that $\gamma = \dots x_{-1}x_0x_1x_2\dots$. Let n be the length of γ. Clearly, $x_i = x_{i+k}$ for all i. So $n \leq 2k$. By Corollary 4.5 n is even, that is, $n = 2m$ for some $m > 0$. This means that $u_j = u_{j+m}$ and $w_j = w_{j+m}$ for all j. It follows that also $v_j = v_{j+m}$, that is, $t_j = t_{j+m}$ for all j. Hence $m \geq k$, giving $n \geq 2k$. Thus, $n = 2k$. $\square$

To conclude this discussion, every zigzag is a boundary zigzag of each of its two side railroads, and similarly, every railroad is a side railroad of each of its two boundary zigzags.

Consider two railroads, $T = \dots t_{-1}t_0t_1t_2\dots$ (with connecting faces T_i) and $S = \dots s_{-1}s_0s_1s_2\dots$ (with connecting faces S_i). We say that T and S *intersect* each other if $T_i = S_j$ for some i and j, and furthermore, $\{t_i, t_{i+1}\}$ and $\{s_j, s_{j+1}\}$ are different pairs of opposite edges on this face.

Since face cycles are isometric, we have the following.

Lemma 4.15. *If two railroads intersect each other then they carry disjoint labels.* $\square$

Since every face F has three pairs of opposite edges, it serves as a connecting face for three railroads. These three railroads intersect one another at F, and so they carry different labels and are pairwise distinct.

We say that two railroads are *neighbours* if they are the two side railroads of the same zigzag.

Lemma 4.16. *Suppose T and S are neighbour railroads. A third railroad intersects T if and only if it intersects S.*

Proof. Suppose a railroad R intersects T at a connecting face T_i. The face T_i is adjacent to two connecting faces of S, say, S_j and S_{j+1}. Manifestly, one of the two railroads intersecting T at T_i intersects S at S_j, and the other intersects S at S_{j+1}. □

We are now approaching the final contradiction. To manufacture this contradiction, we fix a zigzag $\gamma = \dots x_{-1}x_0x_1x_2 \dots$ of length $n = 2k$, where k is the length of the side railroads of γ. Note that since Γ has no 4-cycles, we have $n \geq 6$. Let F_i be the side face of γ at x_i, and let x_iy_i be the side edge at x_i.

Lemma 4.17. *We have that k is even, that is, $k = 2s$ for some s. In particular, $n \geq 8$.*

Proof. The edges x_0x_1 and x_kx_{k+1} are opposite on the zigzag cycle. The latter is isometric by Lemma 4.12, so the two edges above carry the same label. Let T_i be the railroad defined by x_ix_{i+1} and set $T = T_0$. Manifestly, T intersects T_1 at F_1. Furthermore, for every i we have that T_i and T_{i+2} are neighbours. Indeed, they are the side railroads of the zigzag containing $y_{i+1}x_{i+1}x_{i+2}y_{i+2}$. It follows inductively from Lemma 4.16 that T intersects every T_i with odd i.

By the above, T and T_k carry the same label, and so T cannot intersect T_k in view of Lemma 2.1. Thus, k is even. □

Note that $F_k = x_kx_{k+1}y_{k+1}zy_{k-1}x_{k-1}x_k$ for some vertex z. Set $x = x_0$ and consider the following path $\rho = xx_1x_2 \dots x_{k-1}y_{k-1}z$ from x to z. Let us take a look at the labels along this path. First of all, the labels along the subpath from x till x_{k-1} are pairwise disjoint, because the zigzag cycle of γ is isometric. Secondly, $x_{k-1}y_{i-1}$ is a side edge, and so its label is disjoint from all preceding labels. Finally, the edge $y_{k-1}z$ is opposite to x_kx_{k+1} on F_k. So these two edges carry the same label. On the other hand, x_kx_{k+1} is opposite to xx_1 on the zigzag cycle of γ. Hence they also carry the same label. We conclude that $\ell(y_{k-1}z) = \ell(xx_1)$. Combining the labels along ρ, we see that the distance between x and z is $k - 1$, and furthermore, every label on a shortest path from x to z must be contained in

$$\ell(x_1x_2) \cup \dots \cup \ell(x_{k-2}x_{k-1}) \cup \ell(x_{k-1}y_{k-1}).$$

Which edge can come first on the shortest path from x to z? It cannot be xx_1, because its label is disjoint from all the labels in $\ell(x_1x_2) \cup \dots \cup \ell(x_{k-2}x_{k-1})$, because the zigzag cycle is isometric, and disjoint from $\ell(x_{k-1}y_{k-1})$, because $x_{k-1}y_{k-1}$ is a side edge. Similar argument shows that the shortest path cannot start from xx_{n-1}. So the shortest path must start from xy_0. However, this is a side edge, and so its label is disjoint from all labels in $\ell(x_1x_2) \cup \dots \cup \ell(x_{k-2}x_{k-1})$. This means that we must have $\ell(xy_0) = \ell(x_{k-1}y_{k-1})$. According to Corollary 4.4, $k - 1$ is even; a contradiction, since k is even, too. This is our final contradiction and it established for us the following.

Proposition 4.18. *If a polyhex Γ has isometric faces and no 4-cycles then it cannot be ℓ_1.* □

This concludes the proof of our Theorem 1.1.

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