On total coloring of small fullerene nanodiscs

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Abstract. *We investigate the total coloring of fullerene nanodiscs, a subclass of cubic planar graphs with girth* 5 *arising in Chemistry, motivated by a conjecture about the nonexistence of a Type* 2 *cubic graph of girth at least* 5*. We prove an auxiliary lemma which says that every central layer of a fullerene nanodisc is* 4*-total colorable, a necessary condition for the nanodisc to be Type* 1*, and we contribute by giving* 4*-total colorings for small fullerene nanodiscs, showing that these graphs are Type* 1*.*

1. The large girth Type 1 conjecture

A total coloring of a graph G is a color assignment of set $E \cup V$, where E denotes the set of edges and V denotes the set of vertices of the graph, such that adjacent or incident elements have different colors. A k-total coloring of a graph G is a total coloring that uses a set of k colors, and the graph is k-total colorable if it admits a k-total coloring. The total chromatic number $\chi''(G)$ is the smallest natural k for which G is k-total colorable. Behzad and Vizing [Behzad 1965, Vizing 1964] independently conjectured the Total Coloring Conjecture (TCC) that for any simple graph G, we have $\chi''(G) \leq \Delta(G) + 2$. If $\chi''(G) = \Delta(G) + 1$, then the graph is Type 1; if $\chi''(G) = \Delta(G) + 2$, then the graph is Type 2. The TCC has already been settled for cubic graphs [Vijayaditya 1971]. A well-known total coloring result in the literature that establishes the total chromatic number of cycle graphs C_n and that is essential for our results is given by Yap [Yap 1996], and the algorithm that proves this result can be found in Campos' doctoral thesis [Campos 2006].

Theorem 1 ([Yap 1996])**.** *Let* G *be the cycle graph* C_n*. Then* $\chi''(G) = 3$*, if* $n \equiv 0 \mod 3$*; and 4, otherwise.*

Every known Type 2 cubic graph has triangles or squares. So, it is natural to think that there are no Type 2 cubic graphs with girth at least 5. Thus the following conjecture was proposed:

Conjecture 1 ([Brinkmann et al. 2015])**.** *There is no Type 2 cubic graph with girth at least 5.*

Motivated by this conjecture, we investigate the total coloring problem considering cubic planar graphs with large girth that model chemical structures: the fullerene nanodiscs.

2. The fullerene nanodiscs

Fullerene nanodiscs D_r, $r \geq 2$, are mathematical models of carbon-based molecules experimentally found in the early eighties, which are cubic, 3-connected, planar graphs with pentagonal and hexagonal faces. The planar embedding of D_r has its faces arranged into layers, one layer next to the nearest previous layer starting from a hexagonal layer until we reach the other hexagonal layer. The distance between the inner (outer) layer and the central layer, where lie 12 pentagonal faces, is given by the radius parameter $r \geq 2$. Figure 2 shows nanodiscs, where we highlighted with blue color in the central layer the 12 pentagonal faces.

The sequence $\{1, 6, 12, 18, \ldots, 6(r-1), 6r, 6(r-1), \ldots, 18, 12, 6, 1\}$ provides the amount of faces on each layer of the nanodisc graph D_r. The 12 pentagonal faces are distributed in the central layer among its $6r$ faces with the other $(6r - 12)$ hexagonal faces [Nicodemos 2017]. The auxiliary cycle sequence $\{C_6, C_{18}, \ldots, C_{12r-6}, C_{12r-6}, \ldots, C_{18}, C_6\}$ provides the sizes of the auxiliary cycles that define the layers. A nanodisc D_r contains $12r^2$ vertices, $18r^2$ edges and has girth 5.

3. The central layers of fullerene nanodiscs

The first total coloring result in the class of fullerene nanodiscs was established by *da Cruz et al.* in [da Cruz et al. 2021b], showing that the fullerene nanodisc D_2 is Type 1. Note that the number of vertices of every auxiliary cycle of a nanodisc is divisible by 3, and that the radial edges define a perfect matching in D_r, $r \geq 2$. Based on the total coloring algorithm for the cycle graphs provided by the constructive proof of Theorem 1, we are able to prove the following auxiliary lemma that colors the central layer.

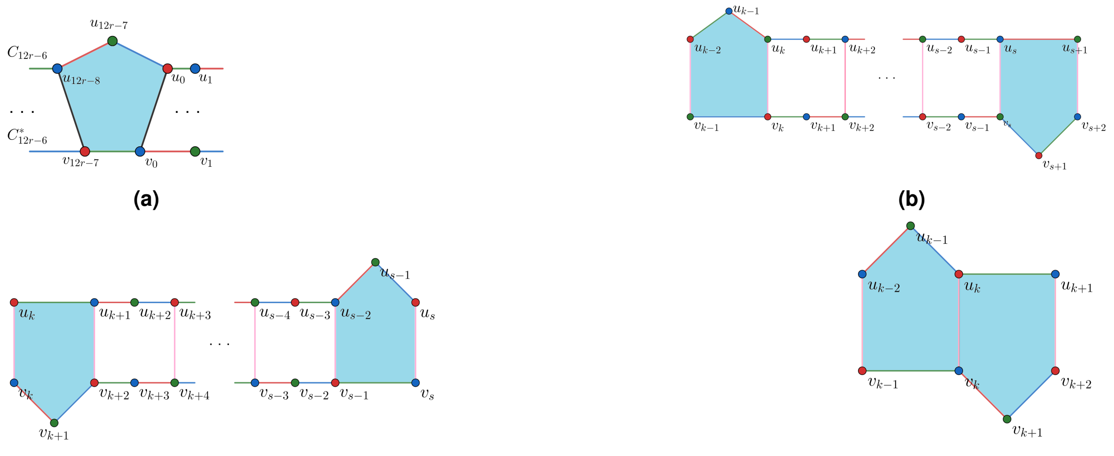


Figure 1. (a) Choice of u_0 and v_0 in C_{12r-6} and C^*_{12r-6}, respectively; (b) Case 1.1; (c) Case 1.2; (d) Case 2.

Theorem 2. *The central layer of every fullerene nanodisc D_r, $r \geq 2$, is 4-total colorable.*

Proof. Let D_r be a nanodisc, $r \geq 2$, and the C_{12r-6} cycles that comprise its central layer. By Theorem 1, there is a 3-total coloring for each C_{12r-6} and an algorithm that provides such coloring [Campos 2006, Yap 1996]. We shall define the cycles and label the vertices of each cycle as follows.

$$V(C_{12r-6}) = \{u_0, u_1, \ldots, u_{12r-7}\}, V(C^*_{12r-6}) = \{v_0, v_1, \ldots, v_{12r-7}\}.$$

Choose u_0 and v_0 such that these vertices are extremes of a pentagonal face, so that the edge u_0v_0 is the second radial edge of this pentagon in a clockwise direction, as illustrated in Figure 1(a). We choose the 3-total coloring for C_{12r-6} by choosing color c_1 for u_0 and for C^*_{12r-6} by choosing color c_3 for v_0. Thus, the color assignment in C_{12r-6} is such that

$$c(u_k) = \begin{cases} c_1, & \text{if } k \equiv 0 \mod 3; \\ c_3, & \text{if } k \equiv 1 \mod 3; \\ c_2, & \text{if } k \equiv 2 \mod 3; \end{cases}$$

$$c(u_k u_{k+1}) = c(u_{k+1}) \mod 3, \ \ \forall u_k u_{k+1} \in E(C_{12r-6}),$$

and for C^*_{12r-6} is such that

$$c(v_k) = \begin{cases} c_3, & \text{if } k \equiv 0 \mod 3; \\ c_2, & \text{if } k \equiv 1 \mod 3; \\ c_1, & \text{if } k \equiv 2 \mod 3; \end{cases}$$

$$c(v_k v_{k+1}) = c(v_{k+1}) \mod 3, \ \ \forall v_k v_{k+1} \in E(C^*_{12r-6}).$$

From the structural results for central layer of D_r obtained in [da Cruz 2022, da Cruz et al. 2021b], it is easy to see that for $r > 2$, there are at most two consecutive pentagons, with balanced hexagons among the groups of pentagons, and the two nearest pentagons are partitioned differently. First, we will check that the radial edges among C_{12r-6} and C^*_{12r-6} are of form u_kv_k or u_kv_{k+1}. To verify this, we must consider two cases of face structure:

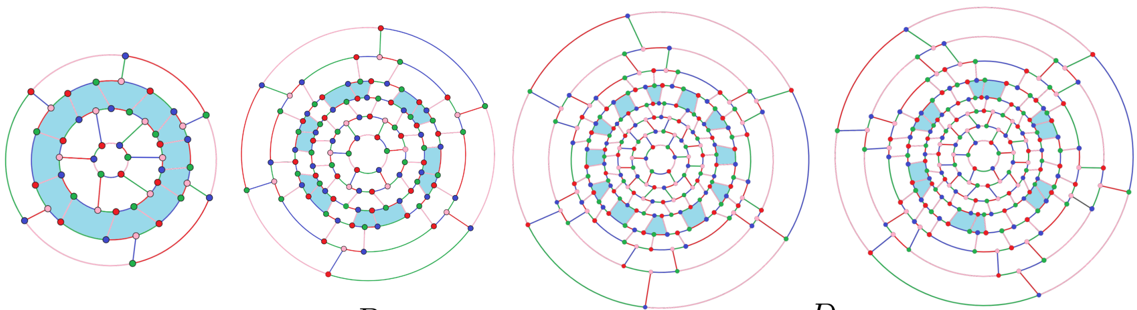
- **Case 1:** There are balanced hexagons besides the two nearest pentagons.
  - **Case 1.1**: The first pentagon has 3 vertices in C_{12r-6}. (See Figure 1(b).) By choice of u_0 and v_0 and by counting vertices, every second radial edge of this pentagon in a clockwise direction is of form u_kv_k, and thus the first radial edge in a clockwise direction is of form u_kv_{k+1}, and every hexagon consecutive to this face will inherit this property. Thus, the hexagonal radial edges are of form u_kv_k. It remains to check the radial edges of the next pentagon. As this pentagon is next in the order to a balanced hexagon, the first radial edge in a clockwise direction is of form u_kv_k. Clearly, the other radial edge is of form u_kv_{k+1}.
  - **Case 1.2**: The first pentagon has 2 vertices in C_{12r-6}. (See Figure 1(c).) As the second radial edge in a clockwise direction is of form u_kv_{k+1}, every hexagon consecutive to this face will inherit this property. Thus, the hexagonal radial edges are of form u_kv_{k+1}. It remains to check the radial edges of the next pentagon. As this pentagon is next in the order to a balanced hexagon, the first radial edge in a clockwise direction is of form u_kv_{k+1}. Clearly, by the structure of these pentagons, the other radial edge is of form u_kv_k.
- **Case 2:** Two consecutive pentagons. (See Figure 1(d).) As the pentagonal structure is preserved, the pentagonal radial edges are of form u_kv_k and u_kv_{k+1}.

It remains to check whether these edges cause color conflict. By the coloring structure, vertices $u_k \in V(C_{12r-6})$ and $v_k \in V(C^*_{12r-6})$ are colored with different classes of colors. Thus, $c(u_k) \neq c(v_k)$ and the edges of form $u_k v_k$ are not in color conflict. Also, by the coloring structure, the colors $c_1, c_2, c_3 \ldots, c_1, c_2, c_3$ are associated in this order with the elements $u_0, u_0u_1, u_1, \ldots, u_{12r-8}u_{12r-7}, u_{12r-8}, u_{12r-7}u_0, u_0$ and the colors $c_3, c_1, c_2, \ldots, c_3, c_1, c_2$ are assigned in this order to the elements $v_0, v_0v_1, v_1, \ldots, v_{12r-8}v_{12r-7}, v_{12r-8}, v_{12r-7}v_0, v_0$.

So note by inspection that $c(u_k) \neq c(v_{k+1})$ and the radial edges of form $u_k v_{k+1}$ are not in color conflict. As none of these radial edges causes a color conflict, just introduce a fourth color class, c_4, in these edges and thus we obtain a 4-total coloring of the central layer for D_r, $r \geq 2$. □

4. Extending the central layer coloring of small fullerene nanodiscs

Based on Lemma 2 and starting from the 4-total coloring obtained for the central layer, we obtained coloring structures that provide the 4-total coloring of the unique non isomorphic representation [da Cruz et al. 2021b] of D_3 and the two non isomorphic instances [da Cruz et al. 2021a] of D_4, proving that these graphs are Type 1. Hence, we have the following result for this class of graphs.



D_2 D_3 D_4

Figure 2. 4-total colorings for small fullerene nanodiscs.

Theorem 3. *The smallest fullerene nanodiscs are Type 1.*

Figure 2 exhibits the 4-total colorings obtained for D_r, $2 \leq r \leq 4$. The 4-total coloring obtained for both instances of D_4 is the same, as both have the same number of vertices, and what differs in the representations of this nanodisc is its central layer. Also, the inner (outer) cycle of D_3 and the two D_4 have the same coloring structure.

The sketch of the proof of these obtained 4-total colorings have been submitted in an article to Matemática Contemporânea 2023.

Current work Theorem 2 gives a 4-total coloring for the central layer of every fullerene nanodisc. We aim to extend Theorem 3 to larger fullerene nanodiscs, proving that D_r, $r \geq 5$, are Type 1, in order to give further evidence to Conjecture 1.

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