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Bilayered cyclofusene

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Abstract Multiply-connected monolayered cyclofusene (MMC) is a fused hexacyclic system with at least two interior empty regions called *holes*. Multiply-connected *bilayered* cyclofusene (MBC) is a structure derived from an *MMC* by replacing each layer of hexacycles by two layers. Various properties of the equitability of these bipartite graphs are examined.

Keywords Multiply-connected bilayered cyclofusene · Equitable · Skewness · Bipartite · Junction

We have previously defined *Cyclofusene* as a corona-condensed benzenoid whose graph-theoretic representation consists of hexacycles each having exactly two non-adjacent shared edges [1–3]. The number of resonance structures in the coronoid hydrocarbons which we termed cyclofusene [3] is well documented [4–6]. Multiply-connected *monolayered* cyclofusene (*MMC*) is defined [7] as a fused hexacyclic system with at least two interior empty regions called *holes*, as in Fig. 1. In this article, we define multiply-connected *bilayered* cyclofusene (*MBC*) as a structure derived from an *MMC* by replacing each layer of hexacycles by two layers, as in Fig. 2a. Let m represent the number of holes in an *MBC*.

As seen in Fig. 2a, each hexacycle must satisfy exactly one of the following:

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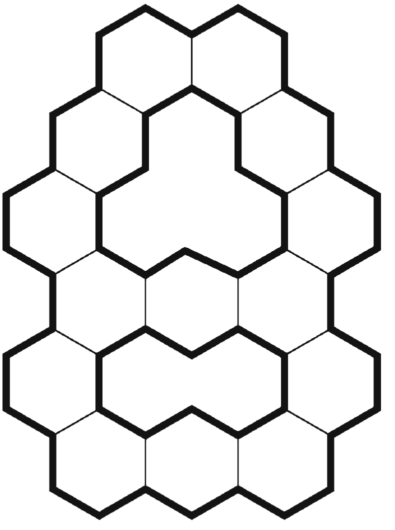


Fig. 1 A multiply-connected monolayered cyclofusene

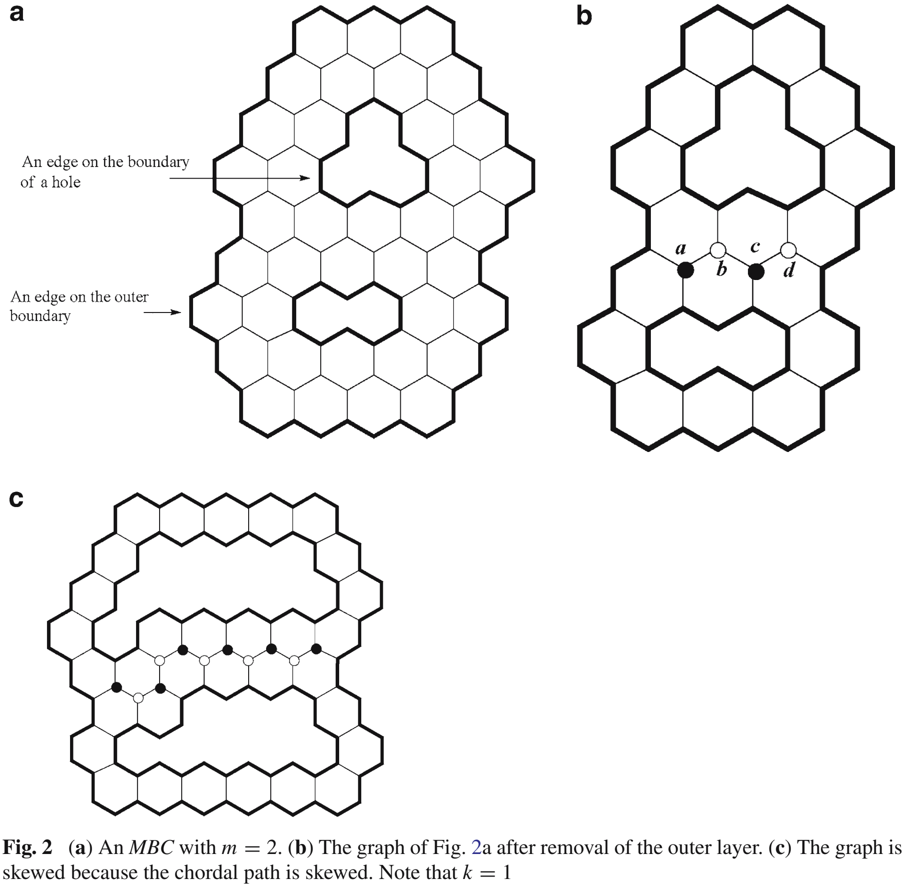


Fig. 2 (**a**) An *MBC* with $m = 2$. (**b**) The graph of Fig. 2a after removal of the outer layer. (**c**) The graph is skewed because the chordal path is skewed. Note that $k = 1$

(a) it has at least one edge on the boundary of exactly one hole, or
(b) it has at least one edge on the outer boundary.

A *perfect matching* is a subset, E, of edges such that each vertex belongs to exactly one edge of E. A bipartite graph is called "equitable" if it has the same number of black and white vertices. Otherwise, define the skewness, k, to be the difference between the number of black and white vertices. If a bipartite graph G has a perfect matching, E, each edge of E joins oppositely colored vertices thereby implying that G is equitable. (Note that even cycles are equitable.) The existence of a perfect matching in a bipartite graph is a necessary condition for aromaticity which requires a distribution of π-bonds each of which is represented by an edge of a perfect matching [1–6]. A further requirement involves the Hückel number $(4n+2)$ which is not pursued here. It should be noted that:

1. all cycles in a bigraph are equitable,
2. paths with oppositely colored endnodes are equitable, and
3. 3-branched star-like trees are equitable if and only if exactly two of the endnodes have the same color as the *junction*, that is, the vertex of degree 3.

As the outer boundary of *MBC* is a cycle, and hence equitable, we shall omit it and its associated layer of hexacycles in order to simplify the figures. Figure 2b illustrates this for the *MBC* of Fig. 2a. In Fig. 2b, the path on vertices a, b, c, and d is denoted a *chordal path*. Since this path is equitable, the entire *MBC* is equitable, that is $k = 0$. In

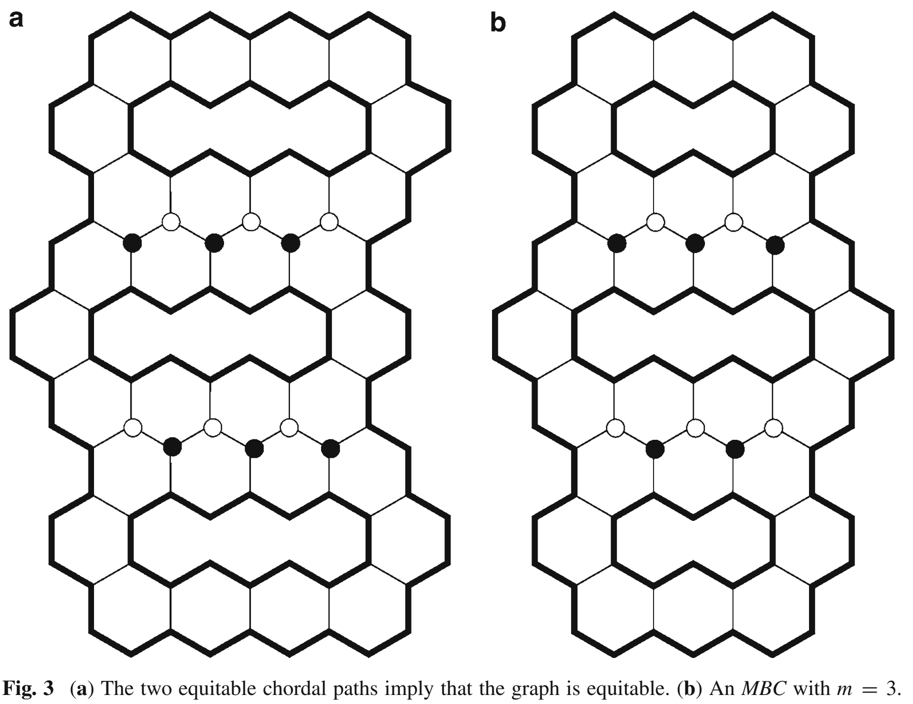


Fig. 3 (**a**) The two equitable chordal paths imply that the graph is equitable. (**b**) An *MBC* with $m = 3$. The two chordal paths are oppositely skewed, so the graph is equitable

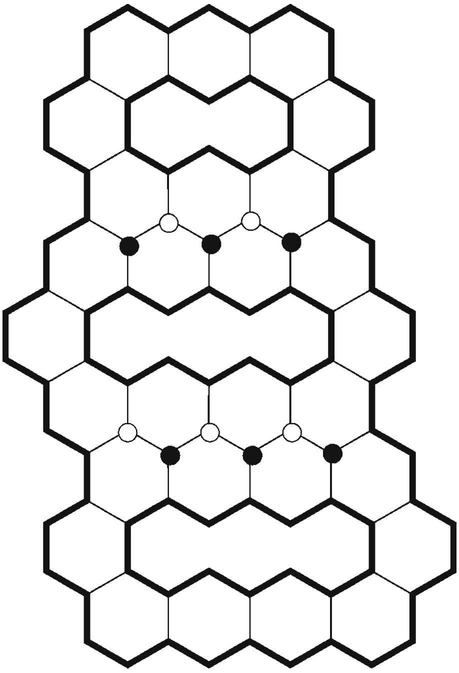


Fig. 4 The upper chordal path is skewed while the lower one is equitable, implying that $k = 1$

Fig. 2c on the other hand, the chordal path is skewed; hence, the graph is not equitable and $k = 1$. Figure 3a depicts an *MBC* with two equitable chordal paths while Fig. 3b depicts two oppositely skewed chordal paths. Both *MBC*s (3a and 3b) are equitable. Contrast this with the *MBC* depicted in Fig. 4 with 3 holes in which $k = 1$ since one chordal path is skewed; hence, the graph is not equitable. In Fig. 5, the two skewed paths favor the same color, so the graph is not equitable, and in fact, $k = 2$.

In an *MBC* with three holes, there are either two disjoint chordal paths as in Figs. 3a, b, 4, and 5 or a 3-branched star-like structure as in Fig. 6a. Structure 6a is equitable since the two endnodes have the same color as the junction.

The following theorems are useful when the number of holes is arbitrary. Denote the number of junctions by j.

Theorem 1 *When adding holes to the graph such that each new junction is connected to the outer cycle, the number of holes and the number of junctions satisfy* $m = j + 2$.

Proof Each new hole is created by only one new junction (termed a *type 1* construction). As the number of holes increments by one, so does the number of junctions. □

Now $j = 2$, $m = 4$ satisfies $m = j + 2$. This relation remains true when m and j are augmented by 1. This can be repeated arbitrarily often (Fig. 6b).

Theorem 2 *When adding holes to the graph such that each new junction is connected to a vertex on another path creating a new junction (two new ones in total), then the number of holes and the number of junctions satisfy* $2m - j = 5$.

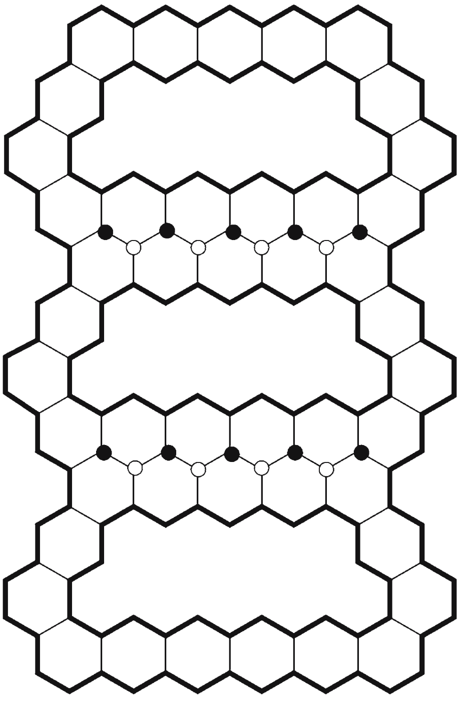


Fig. 5 Both chordal paths are skewed in favor of the same color (black), so $k = 2$ and the graph is not equitable

Proof Each new hole creates two new junctions (termed a *type 2* construction), so the number of junctions increases by two as the number of holes increases by one. □

Now $j = 3$, $m = 4$ satisfies $2m - j = 5$. As in the preceding proof, this remains true after augmenting m and j by 1, or as often as needed (Fig. 6c).

Theorem 3 *When adding holes to the graph, using type 1 and/or type 2 constructions in random succession, we have* $\left\lceil \frac{j+5}{2} \right\rceil \leq m \leq j + 2$.

Proof Maximizing the number of holes corresponding to a fixed number of junctions requires the creation of one junction per hole. This implies exclusive use of type 1 constructions; thereby, justifying $m \leq j+2$ as in Theorem 1. To minimize the number of holes for a fixed number of junctions requires the creation of two junctions per hole. This entails exclusive use of type 2 constructions which in light of Theorem 2 justifies the left inequalities (Fig. 6d). □

The equitability of a type 1 construction (Fig. 6b) is determined by the color of the endnodes and junctions. Each new endnode must be the same color as the corresponding new junction. For example, in Fig. 6b, the endnote x has the same color as the corresponding junction j_3. Toward this end, define the signed skewness of a set of vertices, V, denoted $\mathrm{sk}(V)$, to be the difference in the number of black and white vertices. So if b_V and w_V represent the number of black and white vertices, respectively (in V), then $\mathrm{sk}(V) = b_v - w_v$. In an equitable tree with $\Delta = 3$, we denote the set of

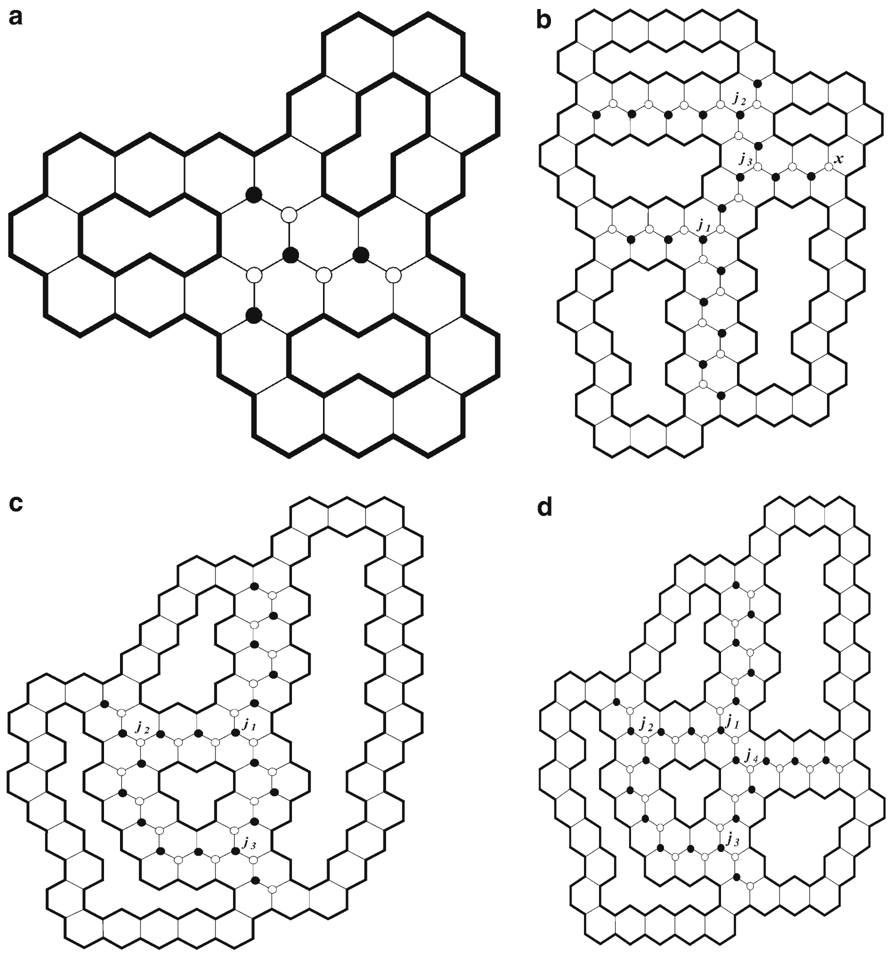


Fig. 6 (**a**) The indicated 3-branched star-like structure is equitable (**b**) Starting with j_1, junctions j_2 and j_3 are added using type 1 constructions. The graph is, therefore, equitable (**c**) The $j_2 - j_3$ path indicates a type 2 construction which preserves equitability since j_2 and j_3 are oppositely colored (**d**) An equitable graph obtained by both types of construction

junctions (vertices of degree 3) by J and the endnodes (vertices of degree 1) by N. The following theorem is relevant to the construction of type 1 structures.

Theorem 4 *For any equitable tree with*

$$\Delta = 3, sk(J) = sk(N). \tag{1}$$

Proof We employ the Junction–Endnode algorithm (JE algorithm) to create equitable trees. Figure 7 depicts an equitable path. Note that (1) is valid because there are no junctions in Fig. 7 and the two endnodes are of opposite color. Note that for simplicity, the remaining vertices on the path are not included.

Fig. 7 An equitable path with only the endnodes represented on the graph

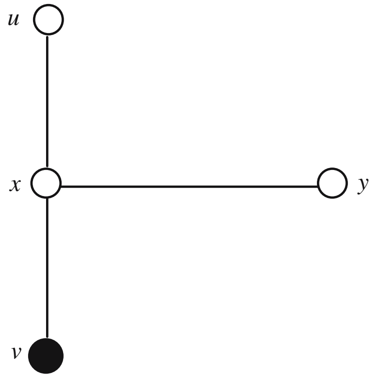


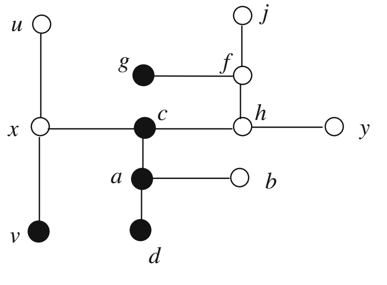
Fig. 8 The original $u - v$ path with path $x - y$ added

Choose an arbitrary vertex on this equitable path and create a path from that vertex. In order to maintain equitability, the endnode of this path must be the same color as the junction, as in Fig. 8.

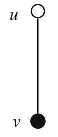
It is important to note that (1) remains valid because the color of the junction is the same as that of the endnode. If the new path ends in an endnode of opposite color, it is necessary that another junction endnode path be created to counter the skewness. Otherwise the tree would no longer be equitable. This need not be done immediately.

The algorithm continues (with the corrective measure when the endnode of a new path has a different color as its associated junction) until the given tree is completed. Since (1) is true at each step, the theorem follows. □

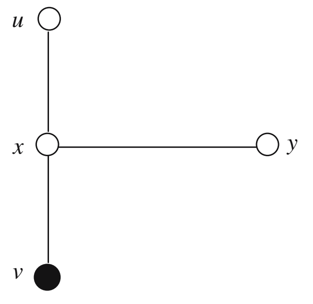
The following example illustrates the JE algorithm.
We wish to construct the following tree:



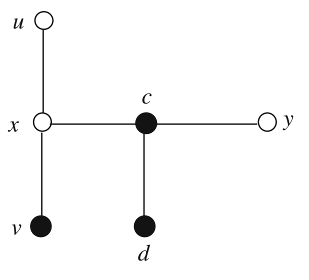
Step 1: Begin with an equitable $u - v$ path:



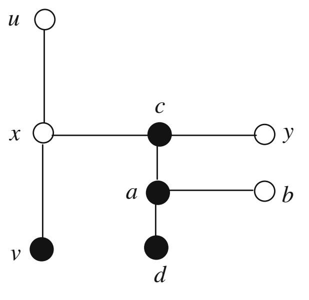
Step 2: Construct path $x - y$ such that x and y have the same color (white):



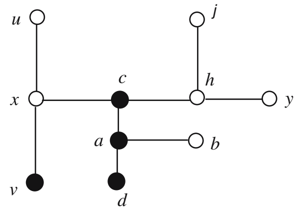
Step 3: Construct path $c - d$ such that c and d have the same color (black):



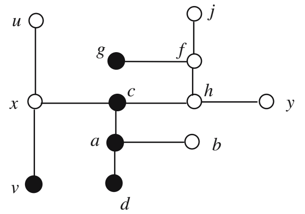
Step 4: Construct path $a - b$ such that a is black and b is white, which will require the corrective measure:



Step 5: Construct path $h - j$ such that the endnode has the same color as the junction:



Step 6: Finally, construct path $f - g$ which will be oppositely skewed to $a - b$ (the corrective measure):



The tree is complete. The cases in which there are more than two layers are under examination.

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