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On the equitability of multiply-connected monolayered cyclofusene

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Multiply-connected monolayered cyclofusene (*MMC*) is a fused hexacyclic system with an exterior region and at least two interior empty regions called *holes*, as in figure 1. Each hexacyle has either: (a) two edges belonging to an exterior boundary and at least one hole, or (b) two edges belonging to boundaries of at least two holes. Let G be the graph of a given MMC. We show that G is equitable if and only if the set of vertices belonging to three hexacycles is equitable.

KEY WORDS: multiply-connected monolayered cyclofusene, equitable, skewness

1. Introduction

Cyclofusene is defined as a corona-condensed benzenoid whose graph-theoretic representation consists of hexacycles each having exactly two non-adjacent shared edges [1–3]. The resonance structure counts in primitive coronoid hydrocarbons, which we termed cyclofusene [3], are well documented [4–6]. *Multilayered cyclofusene* is a fused hexacylic system which can be partitioned into successive layers of cyclofusene [1]. Multiply-connected monolayered cyclofusene (*MMC*), described in this article, is a fused hexacyclic systems with an exterior region and at least two interior empty regions called *holes*, as in figure 1. Furthermore, each hexacyle has either:

(a) two edges belonging to an exterior boundary and at least one hole (see hexacycle A in figure 1), or

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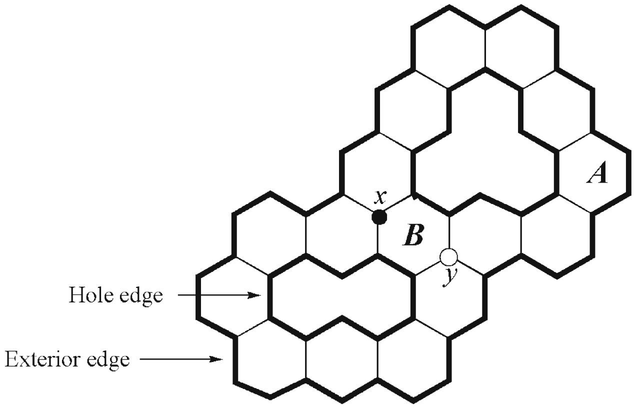

Figure 1. A multiply-connected monolayered cyclofusene with exactly two vertices, x and y, each of which belongs to three hexacycles.

(b) two edges belonging to boundaries of at least two holes (see hexacycle B in figure 1).

Note that some vertices may belong to no boundary cycle. This is because they belong to three hexacycles (see vertices x and y in figure 1. The boundary cycles of the holes and the exterior region are in bold.). Denote by S the set of vertices that do not belong to any of the boundary cycles. In figure 1, $S = \{ x, y \}$, while in figure 2, $S = \{ x \}$.

A graph G is *bipartite* if its vertex set, $V(G)$, can be partitioned into two subsets B and W such that each edge joins a vertex of B with a vertex of W. It is convenient to color the vertices of B and W black and white respectively.

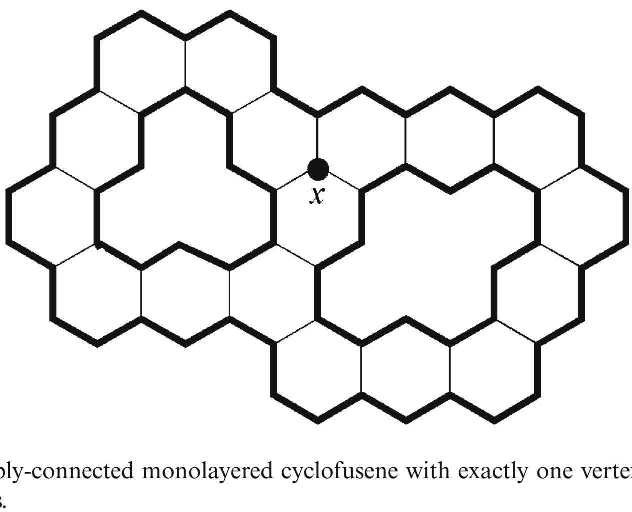

Figure 2. A multiply-connected monolayered cyclofusene with exactly one vertex, x, which belongs to three hexacycles.

If $|B| = |W|$, we call the bipartite graph G *equitable*. If $|B| \neq |W|$, the skewness of G is defined as $| \, |B| - |W| \, |$.

A *perfect matching* is a subset, E, of edges such that each vertex belongs to exactly one edge of E. 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, since the latter implies a distribution of π-bonds each of which is represented by an edge of the perfect matching.

We now present criteria that determine whether or not the graph of a given MMC is equitable. Observe that the boundaries of the exterior region and of the holes of G are bipartite cycles and are, therefore, equitable. It follows, that the union of these boundary cycles is equitable. The vertices of these boundary cycles belong to at most two hexacycles. Hence S, the set of vertices belonging to three hexacycles, is exactly the set of vertices that do not belong to the union of the boundary cycles. It follows that the skewness, k, of S is also the skewness of G. As a result, we have the following theorem:

Theorem 1. Let G be the graph of a given MMC. Then G is equitable if and only if S is equitable.

Proof. A bipartite graph is equitable if and only if the skewness, $k = 0$. Since the skewness of G equals the skewness of S, the theorem follows.

Note that S in figure 1 consists of a black vertex, x, and a white one, y. Then $k = 0$, and the MMC is equitable. On the other hand, figure 2 shows an MMC for which $k = 1$, which indicates that the MMC is not equitable. We end with the following conjectures:

Conjecture 1. Let the graph G of a given MMC have m holes and skewness k. Then $k \leqslant 2m - 2$.

Conjecture 2. Given k and m such that $0 \leqslant k \leqslant 2m - 2$, there exists an MMC with m holes and skewness k. That is, k *interpolates* between 0 and $2m - 2$.

References

[1] S. Karimi and M. Lewinter, J. Math. Chem. 39 (2006) 593–596.
[2] S. Karimi and M. Lewinter, J. Math. Chem. 38 (2005) 103–106.
[3] T. Bocchi, S. Karimi and M. Lewinter, J. Math. Chem. 35 (2004) 339–344.
[4] S.J. Cyvin, B.N. Cyvin, J. Brunvoll, H. Hosoya, F. Zhang, D.J. Klein, R. Chen and O.E. Polansky, Monatsh. Chem. 122 (1991) 435–444.
[5] J. Brunvoll, B.N. Cyvin and S.J. Cyvin, J. Chem. Inf. Comput. Sci. 27 (1987) 14–21.
[6] J. Brunvoll, B.N. Cyvin, S.J. Cyvin, I. Gutman, R. Tosic and M. Kovacevic, J. Mol. Struct. (Theochem.) 184 (1989) 165–177.