Journal of Mathematical Chemistry Vol. 35, No. 4, April 2004 (© 2004)

On the distribution of π bonds in cyclofusene

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Accepted 21 November 2003

We present a type of coronafusene termed cyclofusene, in which each hexacycle shares exactly two nonadjacent edges with other hexacycles. Cyclofusene has exactly four configurations of π bonds such that each π bond belongs to the inner or outer boundary. In each of these configurations, the outer boundary has six more π bonds than the inner boundary. The number of shared π bonds in any mixed configuration is even. Let m be the number of shared π bonds in a mixed configuration for a cyclofusene with exactly k linear chains. Then $m \leqslant k$. Furthermore, there exists a mixed configuration with exactly k shared π bonds.

KEY WORDS: benzenoid, superaromaticity, cyclofusene, dualist graph, perfect matching

AMS subject classification: 05C99

Coronafusene, an abbreviated term used by Balaban [1] to describe corona-condensed benzenoid polycyclic systems, belongs to a class of fused benzenoid hydrocarbons with a cavity. A great deal of attention has been focused on the nomenclature and topological centric coding of these types of *polyhexes* [2–4], as well as the extra stability (superaromaticity) associated with the configuration of π bonds in these super-ring structures [5]. Note that a configuration of π bonds in a fused hexacyclic hydrocarbon corresponds to a perfect matching in its graphical representation [6–14]. In this article, we present a special type of coronafusene which we term *cyclofusene*, in which each hexacycle shares exactly two nonadjacent edges with other hexacycles. Put more simply, the dualist graph of cyclofusene is a cycle.

A hexacycle whose shared edges are not parallel shall be called *type A*. Otherwise it shall be called *type B* (see figure 1). It should be obvious that cyclofusene has at least six A-cycles.

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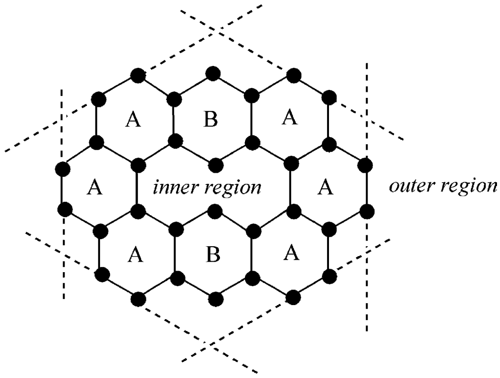

Figure 1. A cyclofusene with labeled hexacycles.

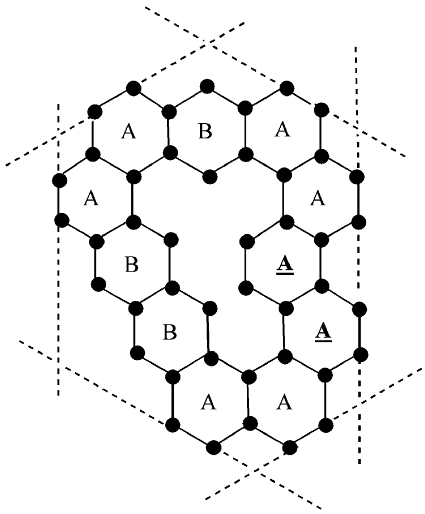

Figure 2. A non-convex cyclofusene and its six support lines.

Observe that there are two regions, inner and outer, of the plane which are not part of the cyclofusene, as shown in figure 1. Two of the four unshared edges of each B-cycle belong to the boundary cycle of the inner region (henceforth called the *inner boundary*) and the other two belong to the boundary cycle of the outer region (the *outer boundary*). On the other hand, a glance at figure 2 shows that the four unshared edges of any A-cycle of a cyclofusene satisfy either:

(1) One edge belongs to the inner boundary and the other three belong to the outer boundary, or
(2) One edge belongs to the outer boundary and the other three belong to the inner boundary.

Observe that in a convex cyclofusene, exactly six A-cycles have an edge on a *support line* – a line through an edge such that the entire cyclofusene lies

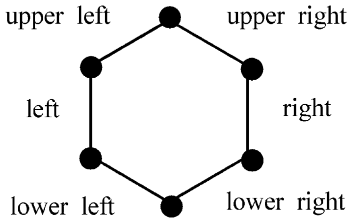

Figure 3. The labeled edges of an A-cycle.

on one side of the line. Cyclofusene has exactly six such support lines. (See figure 1).

Denoting the edges of a hexacycle as in figure 3, as we traverse the hexacycles in a counterclockwise direction, each A-cycle changes our direction by 60° in light of the fact that its shared edges are not parallel. The new direction can be identified by the "pivoting" edge it shares with the hexacycle following it.

In figure 1, the six A-cycles pivot by 60°, respectively, in each of the six directions implied by the labeling of figure 3. This guarantees that we return to the initial hexacycle, thereby forming a "closed" structure. Furthermore, each A-cycle in figure 1 contributes one edge to the inner boundary and three edges to the outer boundary. This can be attributed to the convexity of the inner region. When the inner region is convex, we observe the following:

1. There are six A-cycles.
2. Each A-cycle has one edge on the inner boundary and three edges on the outer boundary.
3. Since each B-cycle contributes the same number of edges (two) to the inner and outer boundaries, it follows that the outer boundary has exactly 12 more edges than the inner boundary.
4. There are exactly six linear chains.

A glance at figure 2 indicates that when the inner region is non-convex,

1. There are more than six A-cycles.
2. Six of these A-cycles are responsible for the six unique pivots that generate the turns which "close" the cyclofusene. These six A-cycles have an edge on a support line.
3. A-cycles in excess of the six A-cycles in #2 occur in pairs (not necessarily consecutive), such that one of the A-cycles has one edge on the inner boundary and three edges on the outer boundary, and the other one has three edges on the inner boundary and one edge on the outer boundary. See the pair of A-cycles in figure 2 labeled with bold, underlined A's.
4. As a result, each pair of A-cycles in #3 contributes an equal number (four) of edges to the inner and outer boundaries.
5. There are more than six linear chains. (The number of linear chains, however, must be even.)

As a result of these observations, we have the following theorems:

Theorem 1. The outer boundary of cyclofusene has 12 more edges than the inner boundary.

Theorem 2. Each of the inner and outer boundaries have an even number of edges.

Corollary. (a) Cyclofusene has exactly four configurations of π bonds such that each π bond belongs to the inner or outer boundary. (b) In each of these configurations, the outer boundary has six more π bonds than the inner boundary.

Proof. A configuration of π bonds corresponds to a perfect matching. Since the boundary cycles are of even order, each of them has two perfect matchings. Then their union has four perfect matchings, each of which corresponds to a configuration of π bonds. By Theorem 1, the outer boundary has twelve more edges than the inner boundary. Since every other edge represents a π bond, part (b) of the corollary is proven. □

A configuration of π bonds such that some of them are shared edges shall be called *mixed*. (No configuration can consist exclusively of shared π bonds, since at least one unshared edge of each six-cycle must be a π bond.) We require the following lemma.

Lemma. Let G be an even cycle from which an odd number of vertices have been deleted. Then G has no perfect matching.

Proof. G has odd order and cannot, therefore, have a perfect matching.

(Note that the above lemma applies if G is obtained by deleting an odd number of vertices from any graph of even order.) We are ready for the following theorem. □

Theorem 3. The number of shared π bonds in any mixed configuration is even.

Proof. A "shared" π bond deletes one vertex from each of the inner and outer cycles. Thus if a mixed configuration had an odd number of shared π bonds, by the above lemma, it would be impossible to complete the "perfect matching" using only edges on the inner and outer boundaries. □

The next theorem presents an upper bound for the number of shared π bonds in a mixed configuration, and shows that this upper bound is always achievable.

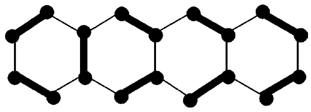

Figure 4. A shared π bond in a linear chain determines the entire configuration and prevents the occurrence of any other shared π bond.

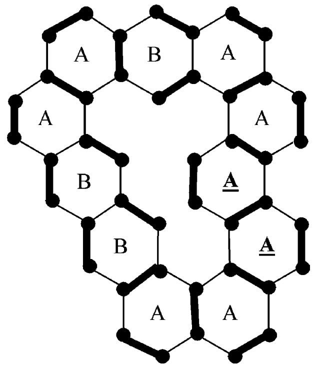

Figure 5. A mixed configuration with $k = 8$ shared π bonds.

Theorem 4. Let m be the number of shared π bonds in a mixed configuration for a cyclofusene with exactly k linear chains. Then $m \leqslant k$. Furthermore, there exists a mixed configuration with k shared π bonds.

Proof. Observe, firstly, that the occurrence of a shared π bond in a linear chain determines the entire configuration and prevents the occurrence of any other shared π bond, (see figure 4), in which the π bonds are denoted by bold edges.

As a consequence, $m \leqslant k$. To show that k is achievable, observe that each linear chain begins and ends with an A-cycle. On the other hand, each A-cycle belongs to two linear chains. It follows that the number of A-cycles is the same as k, the number of linear chains. Now beginning with an arbitrary shared edge, traverse the cyclofusene, say clockwise, and select as a π bond an edge of each encountered A-cycle of each linear chain, resulting in k π bonds. This is illustrated in figure 5 for the cyclofusene of figure 2. □

An integer-valued function, f, on a set $S = \{a_1, a_2, \dots, a_n\}$ is said to *interpolate*, if whenever $f(a_i) < h < f(a_k)$, there exists an element a_j in S such that $f(a_j) = h$. If f assumes only even values, we obtain the *even-interpolation* property by restricting h to even integers.

Let the set S be the configurations of π bonds for a given cyclofusene, and let f be the number of shared π bonds. We conjecture that f has the even-interpolation property.

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