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On the properties of convex multilayered cyclofusene

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Cyclofusene is a corona-condensed benzenoid whose graph-theoretic representation consists of hexacycles each having exactly two non-adjacent shared edges. *Multilayered cyclofusene* is a fused hexacylic system which can be partitioned into successive layers of cyclofusene. In such systems, an edge shared by two consecutive hexacycles in the same layer is termed *radial*. We present upper bounds for the number of radial π-bonds in a convex k-layered cyclofusene.

KEY WORDS: multilayered cyclofusene, corona-condensed benzenoid, radial and boundary edges

Cyclofusene is a corona-condensed benzenoid whose graph-theoretic representation consists of hexacycles each having exactly two non-adjacent shared edges [1–2]. The resonance structure counts in primitive coronoid hydrocarbons, which we termed cyclofusene [1], are well documented [3–5]. Resonance energies in helicinic systems [6] and corannulenes [7] were calculated and predicted these systems to be aromatic. Partitioning of π-electrons in individual benzenoid rings in various types of coronoids were described [8].

Multilayered cyclofusene is a fused hexacylic system which can be partitioned into successive layers of cyclofusene (figure 1). In such systems, an edge shared by two consecutive hexacycles in the same layer is termed *radial*, while all other edges are called *boundary*. A cycle (other than a hexacycle) consisting exclusively of boundary edges is called a *boundary cycle* (figure 1).

A *convex* multilayered cyclofusene (CMC) contains exactly six global support lines that determine a convex hexagon. This can be accomplished in two different ways, one emphasizing the six pivot cycles of the outer layer (figure 2a), the other emphasizing the vertices of the outer boundary (figure 2b). A *linear chain* is a sequence of hexacycles in the same layer whose dualist graph is a path,

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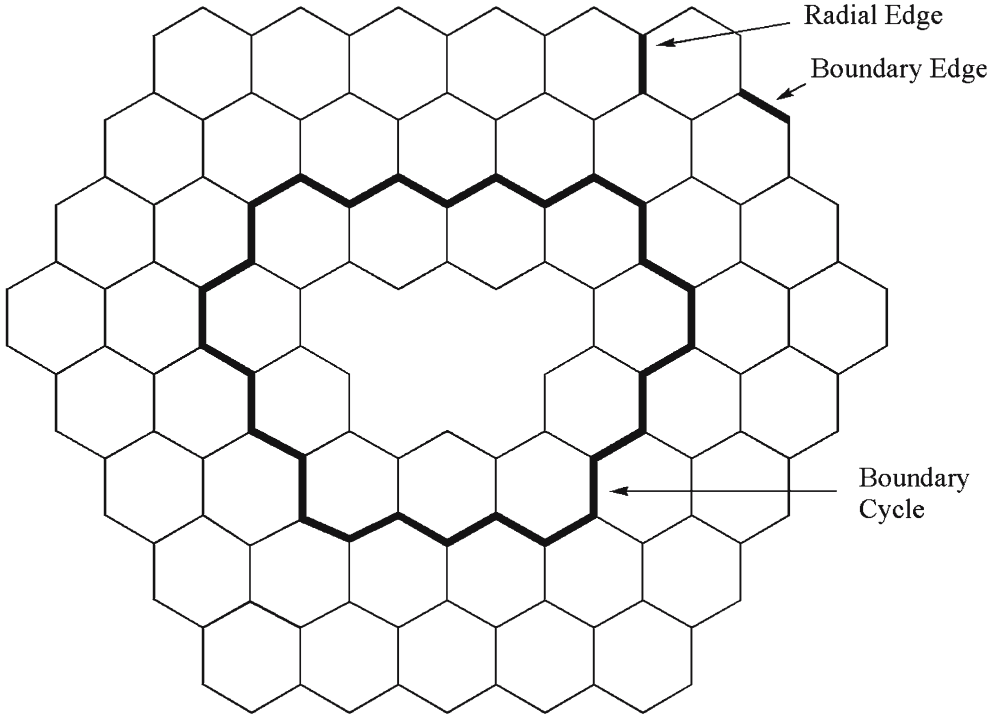

Figure 1. A multilayered cyclofusene showing a radial and a boundary edge and a boundary cycle.

and whose initial and final hexacycles are pivot cycles (called A-cycles in reference 2), i.e., hexacycles whose shared edges in the linear chain are not parallel (figure 2b).

As we proceed from a linear chain in a given layer to the corresponding linear chain in the next layer (moving outward), we acquire a single additional hexacycle contributing to two additional boundary edges. As this happens six times (each layer in CMC has six linear chains), the total increment in boundary edges is twelve. Moreover, the additional hexacycle introduces exactly one new radial edge resulting in an increment of six radial edges for the entire new layer.

Note that if there are k-layers, there are $k+1$ boundary cycles. It follows that a k-layered cyclofusene has exactly 2^{k+1} configuration of π-bonds such that each π-bond is a boundary edge, that is, a *boundary π-bond*. We turn our attention to configurations that contain boundary and radial π-bonds.

Theorem 1. Given a k-layered CMC, the upper bound for the number of radial π-bonds is $6\left\lceil \frac{k}{2} \right\rceil^2$ when k is odd, and $\frac{3}{2}\left(k^2+2k\right)$ when k is even.

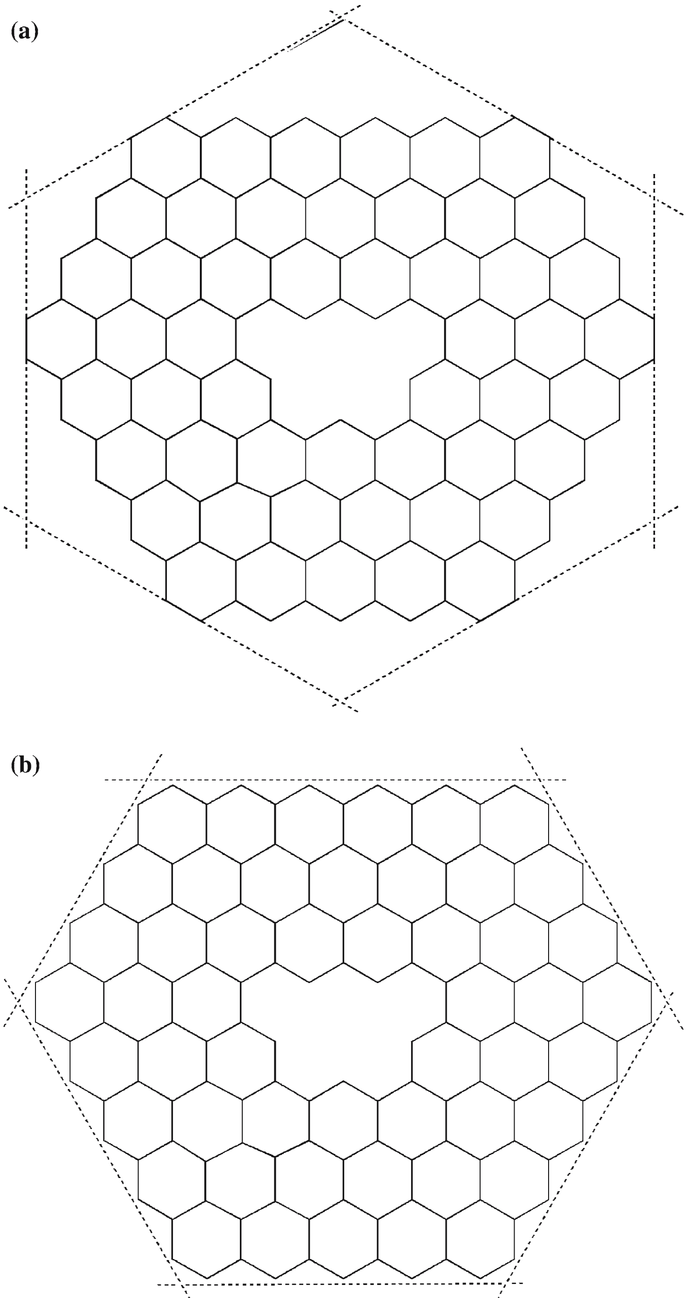

Figure 2. (a) Support lines emphasizing the six pivot cycles of the outer layer. (b) Support lines emphasizing the vertices.

Proof. Label the layers of CMC 1 through k, respectively, and observe using the proof of theorem 4 in reference 1 that the linear chains of layers 1 and k can have at most one radial π-bond each. A glance at figure 1 shows that layers 2 and $k-1$ can have at most two radial π-bonds per linear chain. Similarly, layers 3 and $k-2$ can have at most three radial π-bonds per linear chain. This process terminates in one of the following two cases.
Case 1. k is odd. The terminal layer $\lceil \frac{k}{2} \rceil$ can have at most $\lceil \frac{k}{2} \rceil$ radial π-bonds per linear chain.
Case 2. k is even. The two consecutive terminal layers $\frac{k}{2}$ and $\frac{k}{2}+1$ can have at most $\frac{k}{2}$ radial π-bonds per linear chain.
We now obtain global bounds for the number of radial π-bonds for a k-layered CMC. There are two cases:
Case 1. k is odd. As there are six linear chains per layer we obtain

$$6\left(1+2+3+\cdots+\left\lceil \frac{k}{2} \right\rceil+\cdots+3+2+1\right)=6\left\lceil \frac{k}{2} \right\rceil^{2}.$$

Case 2. k is even. We no longer require the round-down, but we must take into account the second *middle* layer. We obtain

$$6\left(\frac{k}{2}\right)^{2}+6\left(\frac{k}{2}\right)=\frac{3}{2}\left(k^{2}+2k\right).$$

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