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Interpolation of shared π-bonds in cyclofusene

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Cyclofusene is a corona-condensed benzenoid whose graph-theoretic representation consists of hexacycles with exactly two non-adjacent shared II-bonds. We showed that the number of linear chains, k, is an upper bound for m, the number of shared II-bonds. Furthermore, this upper bound is achievable. In this paper, we show that given a positive even integer $m < k$, there exists m shared II-bonds. In other words, the number of shared II-bonds in cyclofusene has the even interpolation property.

KEY WORDS: cyclofusene, graph-theoretic, hexacycles, corona-condensed benzenoid, interpolation

The resonance structure counts [1,2] in primitive coronoid hydrocarbons, termed "Cyclofusene" [3], has been extensively studied [4–6]. We have previously shown [3] that given a mixed configuration of cyclofusene with k linear chains containing m shared II-bonds, m is even and $m \leqslant k$. Furthermore, the case $m = k$ is achievable. We conjectured [3] that the number of shared II-bonds in a given cyclofusene, has the even interpolation property [7] on the set of configurations of that cyclofusene. In this paper, we verify this conjecture by defining the following operation:

Let f be an integer-valued function with domain $\{n_1, n_2, \ldots, n_r\}$. f *interpolates* if whenever a given integer h satisfies the inequality $f(n_i) < h < f(n_k)$, there exists an element n_j in the domain such that $f(n_j) = h$. If f is even-valued, we have the even interpolation property upon restricting h to even integers.

Given a cyclofusene, let e be a shared π-bond in a linear chain with end cycles α and β, as in figure 1. Note that the remaining shared π-bonds in the linear chain are determined by the location of e. We define a "push of the shared π-bond e toward the pivot cycle β" as the sequence depicted by figures 1–3.

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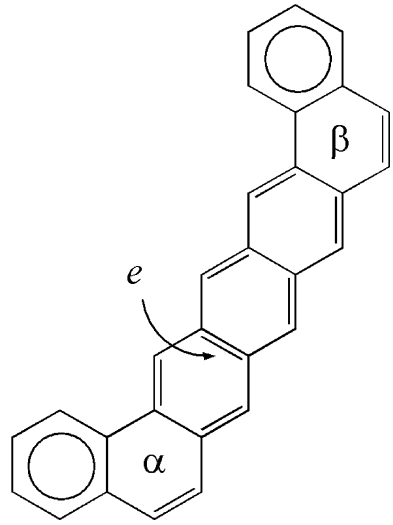

Figure 1. A cyclofusene with a shared π-bond in a linear chain.

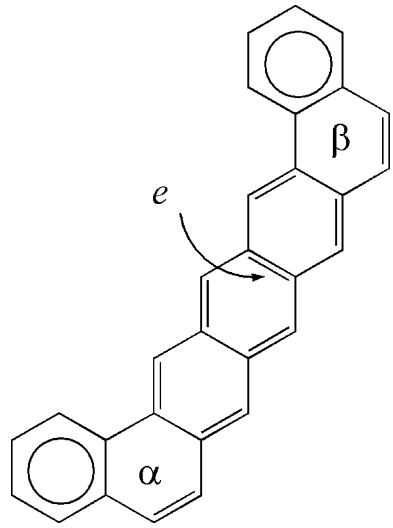

Figure 2. The first push of the shared π-bond toward the pivot cycle β.

Let G be the graph-theoretic representation of a cyclofusene with k linear chains and k shared π-bonds. Using two "pushes" of the shared π-bonds of two consecutive linear chains, we can move both shared π-bonds to the pivot cycle A of the two linear chains as in figure 4. Upon delocalizing the π-bonds of pivot cycle A, we obtain a pivot cycle with no shared π-bonds. That is, the two "pushed" π-bonds have been eliminated, thereby lowering the number of shared

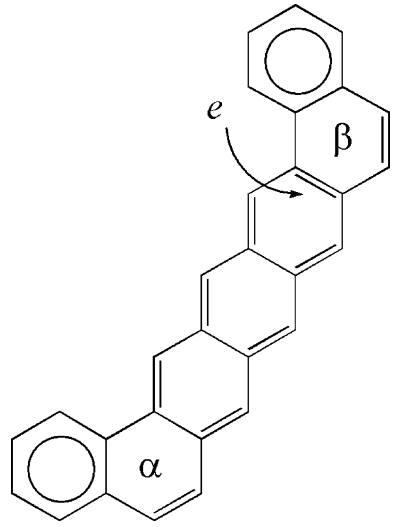

Figure 3. The second push of the shared π-bond toward the pivot cycle β.

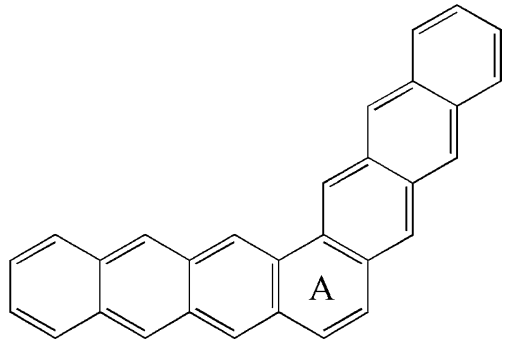

Figure 4. Both shared π-bonds are pushed to the pivot cycle A.

π-bonds in G from k to $k-2$. Upon repetition of this procedure as often as required, we obtain the following theorem:

Theorem. Given a cyclofusene G with k linear chains, the number of possible shared π-bonds has the even interpolation property between 0 and k.

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