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Structural Fusion of Condensed Benzenoid Systems

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On the basis of ring topologies, some theorems for the structural fusion of condensed benzenoids are presented. It has been proved that the oddness or evenness of the fused system is dictated by the degree of fusion.

Introduction

Benzenoid hydrocarbons form an important and well investigated class of conjugated compounds. Benzenoid graphs are the networks obtained by arranging congruent regular hexagons in the plane so that two hexagons are either disjoint or possess a common edge[1].

The concept of all-benzenoid hydrocarbons was introduced by Clar and Zander [2], and eloboration on it eventually led to the formulation of Clar's well known aromatic sextet theory[3].

Actually there exist many publications on the theory of benzenoid hydrocarbons[4–11], and a good account of topological properties of benzenoid systems is presented by Gutman[12].

Although in the last decade there have been innumerable articles on the structural theory of benzoid hydrocarbons, some of which are cited above, there is still more to be investigated. In the present study, some light has been shed on the fusion of condensed benzonoid systems.

Theory

Structural Fusion of Benzenoid Systems

Theoretically, a large benzenoid system can be regarded as resulting from the fusion of two or more smaller benzenoid systems. The process of fusion in that sense requires the overlap of a certain number of edges and vertices of the corresponding molecular graphs of the systems being considered.

Let V_1 and V_2 be vertex sets of benzenoid graphs G_1 and G_2, respectively, such that

$$V_1 = \{v_i \, : \, v_i \, \varepsilon \, V_1\} \tag{1}$$

$$V_2 = \{v_j \, : \, v_j \, \varepsilon \, V_2\} \tag{2}$$

Definition 1: The degree of fusion (DF) of either of benzenoid graphs G_1 and G_2 (geneating graphs) in the prosses of fusion is given by $DF = V_1 \cap V_2$, where V_1 and V_2 are the corresponding vertex sets.

Note that in general the fusion of two-ring systems associated with $DF = 1$ yields a spiro compound, the possibility of which is excluded in the case of benzenoid compounds.

In the case of condensed benzenoid systems, an individually fused ring may have a DF of 2-6. In the present study, such rings are denoted as R_2, R_3, R_4, etc. Figure 1 depicts some R_3- and R_4- type rings present in benzopyrene.

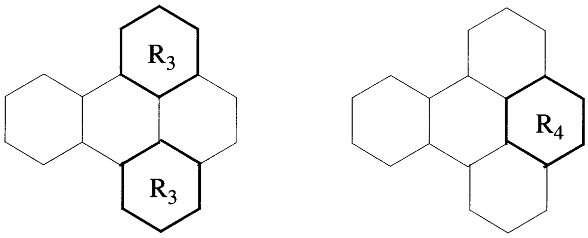

Figure 1. R_3- and R_4- type rings of benzopyrene

Let G_1 and G_2-be two benzenoid graps and F_i be an i-type fusion operator that operates on G_1 and G_2 to produce a larger graph, G, which possesses m of R_i-type rings. The whole fusion process can then be represented as

$$F_i(G_1, G_2) = G(mR_i) \tag{3}$$

The topologies of the simple and the complex type R_3 rings obtained from anthracene system are shown in Figure 2, whereas some R_4-type rings are depicted in Figure 3. Note that various fissures and bays[8] are involved in the formation of R_3- and R_4-type rings, respectively.

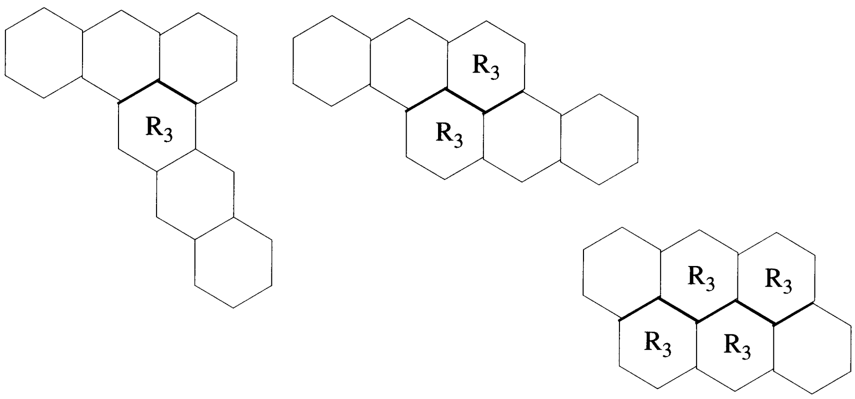

Figure 2. Topologies of R_3-type rings obtained from anthracene

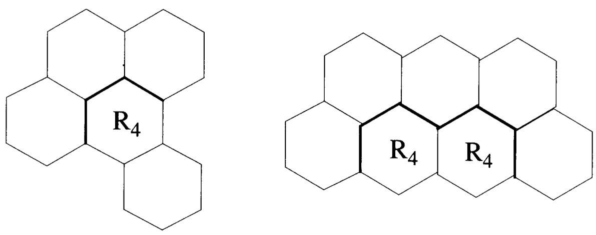

Figure 3. Topologies of R_4-type rings

Superimposition of Benzenoid Systems

Definition 2: The process in which one or more rings of two benzenoid graphs overlap is called superimposition.

Definition 3: The number of benzenoid rings overlapped in the process of superimposition is called the degree of superimposition (DS).

The superimposition operator, S_{ij}^{DS} (where i and j stand for the number of benzenoid rings present in graphs G_i and G_j, respectively, and DS is the degree of superimposition) engenders larger benzenoid graphs starting with smaller members. Figure 4 depicts some superimposition patterns of naphthalene obtained by the overlap of another naphthalene system, and shows the ring topologies[13] of the resultant cata-condensed systems as well. Note that isomeric systems

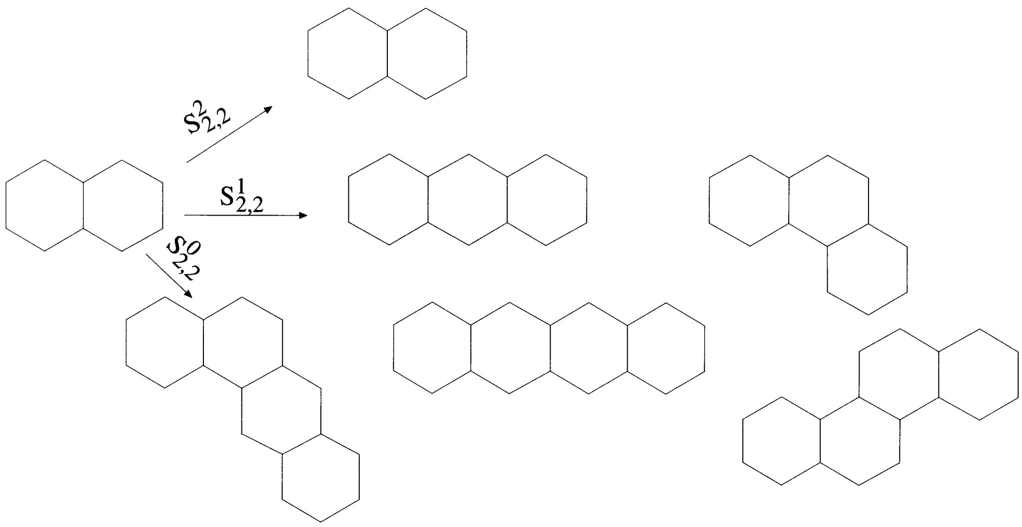

Figure 4. Some superimposition patterns of naphthalene

are produced by the same superimposition operator. In general, the number of benzenoid rings (R) in the final system is given as

$$R = i + j - DS \tag{4}$$

Hence, cata-condensed benzenoids produced by the same superimposition operator are evidently isomers of one another.

Theorem 1. Let G_1 and G_2 be any two add alternant benzenoid graps. If the fusion of G_1 and G_2 to produce graph G is accompanied by the emergence of an even (odd) number of simple R_3- type rings, then G is an even (odd) alternant system.

Proof. Let v_1, v_2 and v be the number of vertices in graphs G_1, G_2 and G, repectively. Since G_1 and G_2 correspond to odd alternant hydrocarbons, suppose $v_1 = 2k + 1$ and $v_2 = 2t + 1$ where k and t are any integers. Since the presence of every simple R_3-type ring means three vertices of G_1 and G_2 are mutually shared to produce graph G, which is $F_3(G_1, G_2) = G(mR_3)$, then

$$v = v_1 + v_2 - 3m \tag{5}$$

where m is the number of R_3-type rings. Inserting the above parametric forms of v_1 and v_2 into equation (5), one obtains

$$v = 2k + 2t + 2 - 3m \tag{6}$$

Note that the degree of fusion in this case is equal to 3m. Since $2(k + t + 1)$ is an even number, the oddness or evenness of v is dictated directly by the parity of m; that is, if m is even (odd) then v is even (odd), which proves the theorem. Below, figure 5 illustrates the application of Theorem 1.

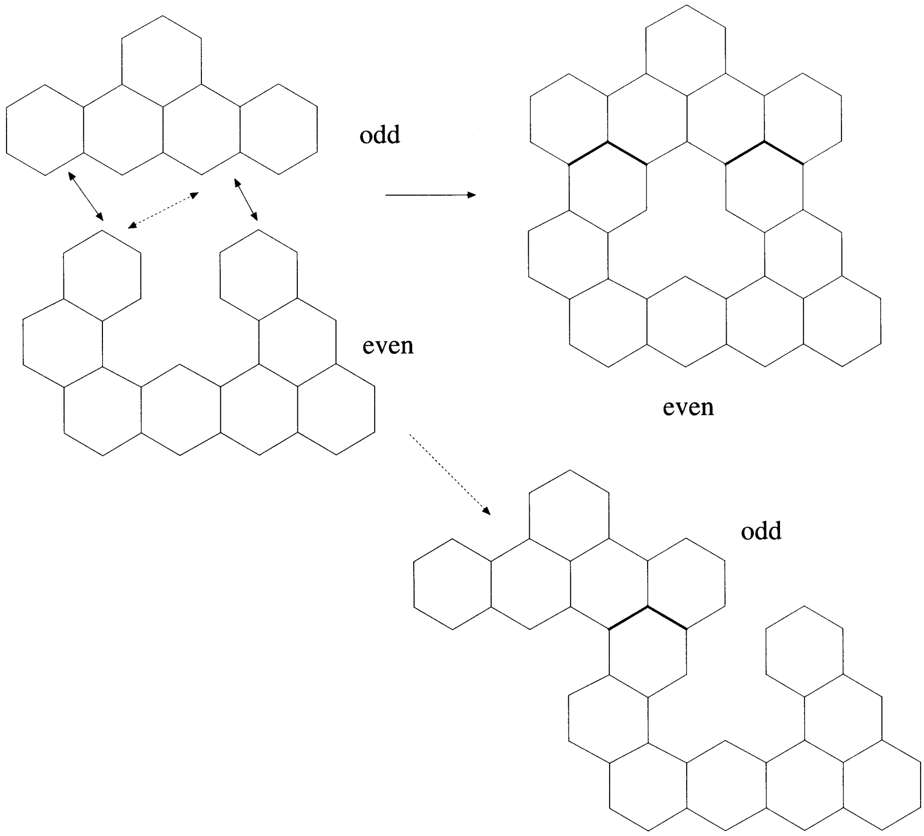

Figure 5. The fusion of two odd benzenoid systems

Corollary 2. Let G_1 and G_2 be any odd even benzenoid graphs, respectively. If an even (odd) number of simple R_3-type rings appears in the fusion process of G_1 and G_2 to produce graph G, then G is an odd (even) alternant system.

Corollary 3. Let G_1 and G_2 be any two even benzenoid graphs. If their fusion to produced graph G is accompanied by the emergence of an even (odd) number of simple R_3-type rings, then G is an even (odd) alternant system.

Corollary 4. If the fusion of any two add (even) benzenoid graphs G_1 and G_2 is accompanied by the emergence of any number of simple R_4-rings, then the resultant graph, G, is an odd (even) alternant system.

Corollary 5. Let G_1 and G_2 be any odd and even benzenoid graphs, respectively. If the fusion of G_1 and G_2 to produce graph G results in any number of simple R_4-type rings, then G is an odd alternant system.

Definition 4. In the process of the fusion of graphs G_1 and G_2, the mutually shared vertices are called the fusion points. Note that the total number of fusion points is equal to DF.

Corollary 6. Let G_1 and G_2 be any odd or even benzenoid graphs. If the number of fusion points between them is odd (even), then the combined graph G obtained by the fusion of G_1 and G_2 is an odd (even) alternant system.

Corollary 7. Let G_1 and G_2 be any odd and even benzenoid graphs, respectively. If the number of fusion points between them is odd (even), then the combined graph G obtained by the fusion of G_1 and G_2 is an even (odd) alternant system Figure 6).

Conclusion

The results of the preceeding section offer a straightforward method for the structural recognition of benzenoid hydrocarbons, and it is perfectly suited to the generations, searches and classification of benzonid systems. The present theorems shed some light on how variations in the structural fusion of components dictate the oddness or evenness of the benzenoid hydrocarbons; thus, certain properties of alternant hydrocarbons, such as the existence of nonbonding molecular orbitals, can be considered componentwise. Obviously, investigations into how fused systems affect certain other theoretical and physico-chemical properties of the combined systems would make very interesting future studies.

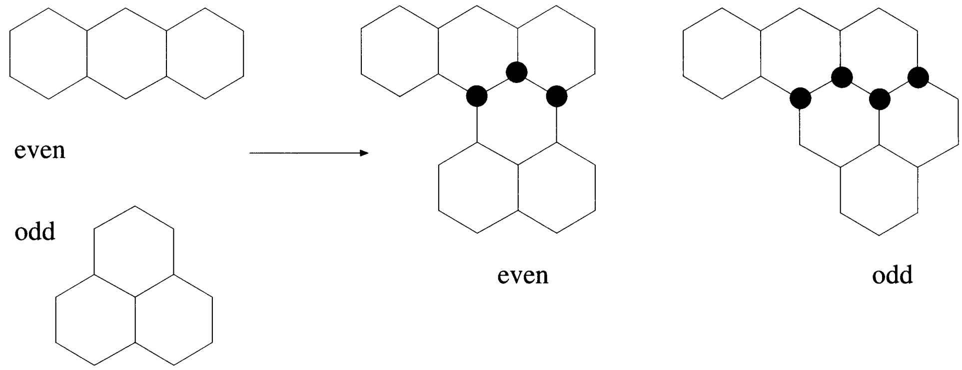

Figure 6. The fusion of an odd and an even benzenoid systems

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