# Cycles in Dicyclopenta–Derivatives of Benzenoid Hydrocarbons

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## Abstract

Let $n_+(G)$, $n_-(G)$, and $n_0(G)$ be the number of positive, negative, and zero eigenvalues of the graph $G$. If $G$ represents the carbon–atom skeleton of a conjugated molecule then, within the Hückel molecular–orbital model, $n_+(G)$, $n_-(G)$, and $n_0(G)$ are the numbers of bonding, antibonding, and non-bonding molecular orbitals. Whereas for Kekuléan benzenoid systems and their monocyclopeta–derivatives, $n_+ = n_-$ and $n_0 = 0$, this is not always the case with their dicyclopenta–derivatives. Let $D$ be the molecular graph of a dicyclopenta–derivative of a benzenoid hydrocarbon. In order to elucidate the structural requirements for the validity of $n_+(D) > n_-(D)$, it is necessary to analyze the cycles of $D$. Let $Z$ be a cycle of $D$ and $|Z|$ its size. We show that if $Z_{AB}$ is a cycle, embracing both five-membered rings of $D$, then $n_0(D - Z_{AB}) = 0$ happens only if $|Z_{AB}| \equiv 0 \ (mod \ 4)$. If $Z_A$ and $Z_B$ are disjoint cycles, embracing the two five-membered rings of $D$, then $n_0(D - Z_A - Z_B) = 0$ happens only if $|Z_A| + |Z_B| \equiv 2 \ (mod \ 4)$.

## INTRODUCTION

Within the Hückel molecular orbital (HMO) model, Kekuléan benzenoid hydrocarbons have equal number of bonding and antibonding MOs, and have no non-bonding MO. Continuing our systematic studies of cyclopenta–derivatives of benzenoid hydrocarbons [1], we found that in these conjugated systems such distribution of MOs may be either preserved or violated, depending on the number and position of the five–membered rings [2–6]. Some general regularities along these lines were recently established [7]. In particular, the problem was completely solved in the case of Kekuléan monocyclopenta– as well as in *syn*-dicyclopenta–derivatives: these have equal number of bonding and antibonding MOs, and no non-bonding MO. In *anti*-dicyclopenta–derivatives, the number of bonding MOs may exceed that of the antibonding MOs. In [7] a sufficient condition for this was found, namely

$$K(B)^2 + K(B-p-q-r-s)^2 < 4 \sum_A \sum_B K(D-Z_A-Z_B)^2 + 2 \sum_{AB} K(D-Z_{AB})^2 \quad (1)$$

where the notation will be explained below. The aim of the present paper is to offer a full derivation of Eq. (1). In order to achieve this goal, the cycles of the dicyclopenta–derivatives need to be duly examined.

We first repeat a few well known graph–theoretic properties of molecular graphs and specify our notation [8, 9].

Let $G$ be the graph representing the carbon–atom skeleton of a conjugated hydrocarbon (a so-called Hückel graph) [8–10]. Let $G$ possess $n$ vertices, and let its spectrum consist of the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. As well known [8–10], these eigenvalues are closely related to the Hückel molecular orbital (HMO) energy levels of the underlying conjugated $\pi$-electron system. Let $n_+ = n_+(G)$, $n_- = n_-(G)$, and $n_0 = n_0(G)$ be the number of eigenvalues of $G$ that are, respectively, positive, negative, and equal to zero; of course, $n_+ + n_- + n_0 = n$. In HMO theory, $n_+$, $n_-$, and $n_0$ are the number of bonding, antibonding and non-bonding MOs [8–10].

Let $e$ be an edge of the graph $G$, connecting the vertices $u$ and $v$. Let $Z$ be a cycle of $G$ in which the edge $e$ is contained. Then the characteristic polynomial of $G$

satisfies the recurrence relation [9, 11, 12]

$$\phi(G, \lambda) = \phi(G - e, \lambda) - \phi(G - u - v, \lambda) - 2 \sum_Z \phi(G - Z, \lambda) \qquad (2)$$

with the summation going over all cycles $Z$ containing the edge $e$; if the graph $G$ has no such cycles, then $\sum_Z \phi(G - Z, \lambda) \equiv 0$.

Denote by $\mathbf{A}(G)$ the adjacency matrix of the graph $G$. Since, by definition [9], $\phi(G, \lambda) = \det[\lambda \mathbf{I} - \mathbf{A}(G)]$, we immediately get $\phi(G, 0) = (-1)^n \det \mathbf{A}(G)$, from which it follows

$$\phi(G, 0) = (-1)^n \prod_{i=1}^{n} \lambda_i . \qquad (3)$$

The following immediate consequence of Eq. (3) will be needed in the subsequent considerations:

**Lemma 1.** *Let $G$ be a graph with even number of vertices, and without zero eigenvalues. If*

$$(-1)^{n/2} \phi(G, 0) < 0 \qquad (4)$$

*then $n_+(G) \neq n_-(G)$. If $G$ is the molecular graph of a $\pi$-electron systems, then inequality (4) implies that the numbers of bonding and antibonding MOs are different.*

One should note that (4) is a sufficient, but not a necessary condition for the non-equality of the numbers of bonding and antibonding MOs, i. e., for $n_+(G) \neq n_-(G)$. In particular, if $n_+ = n/2 \pm 2k$ for some $k \geq 1$, then the inequality (4) will not hold. The chemically most relevant case is when $n_+ = n/2 \pm 1$. Then inequality (4) is both necessary and sufficient.

Most of the graphs encountered in this work are bipartite. If $G$ is a bipartite graph, then its vertices can be colored by two colors (say, black and white), so that the colors of adjacent vertices are always different. In Fig. 1 are depicted two benzenoid graphs and the coloring of their vertices indicated.
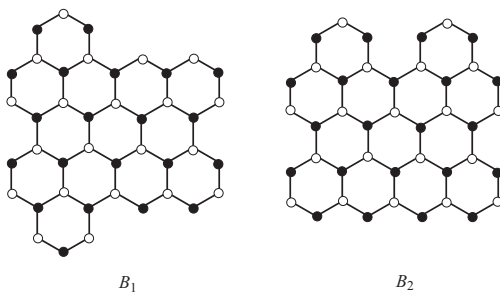
**Fig. 1.** Two benzenoid systems with colored vertices. In the theory of benzenoid systems it is customary that the peak vertices are colored white and the valley vertices black. The graph $B_1$ has 21 black and 21 white vertices, and therefore its color excess is zero. The graph $B_2$ has 22 black and 20 white vertices and its color excess is 2.

Let the vertices of $G$ be colored so that $n_b$ of them are black and $n_w$ are white; $n_b + n_w = n$. Then $CE = CE(G) = |n_b - n_w|$ is called the color excess of $G$. For example, for the graphs depicted in Fig. 1, $CE(B_1) = 0$ and $CE(B_2) = 2$.

If the color excess of a bipartite graph $G$ is different from zero, then this graph has at least one zero eigenvalue. Consequently, we have:

**Lemma 2.** *If the color excess of a bipartite graph $G$ is greater than zero, then the product of all eigenvalues of $G$ is equal to zero, and by Eq. (3), $\phi(G, 0) = 0$.*

The eigenvalues of a bipartite graph $G$ obey the pairing theorem, namely $\lambda_i = -\lambda_{n+1-i}$ holds for all $i = 1, 2, \ldots, n$. This implies that $n_+(G) = n_-(G)$.

Let us now focus our attention to benzenoid hydrocarbons [13, 14]. Let $B$ be the molecular graph of a benzenoid system. This graph is bipartite and therefore Lemmas 2 and 3 are applicable to it. Moreover, according to the famous Dewar–Longuet–Higgins formula [15],

$$\phi(B, 0) = \det \mathbf{A}(B) = (-1)^{n/2} K(B)^2 \tag{5}$$

where $K(B)$ is the Kekulé structure count [14, 16], and where, as before, $n$ is the number of vertices of $B$. [14, 16]. It has been shown [17] that Eq. (5) applies also to subgraphs obtained by deleting from $B$ either non-internal vertices or cycles or both.

It is worth noting that if a graph $G$ satisfies the Dewar–Longuet–Higgins formula, then $n_0(G) = 0$ if and only if $K(G) > 0$.

In what follows we shall be interested only in Kekuléan benzenoids (those possessing at least one Kekulé formula structural, $K(B) > 0$). If so, then $n$ is necessarily even, and $CE(B) = 0$. For instance, one of the benzenoid systems depicted in Fig. 1 has zero color excess and is Kekuléan, $K(B_1) = 175$, whereas the other has non-zero color excess and is non-Kekuléan, $K(B_2) = 0$.

A simple corollary of Eq. (5) is that if $B$ is a Kekuléan benzenoid system, then $n_+(B) = n_-(B) = n/2$ and $n_0(B) = 0$. In other words, within the HMO approximation, a Kekuléan benzenoid molecule has equal number of bonding and antibonding MOs and has no non-bonding MO.

## TOPOLOGICAL PROPERTIES OF DICYCLOPENTA–DERIVATIVES OF BENZENOID HYDROCARBONS

In the case of dicyclopenta–derivatives of benzenoid hydrocarbons we must distinguish between two cases. We refer to them as *syn* and *anti*.

Two cyclopentadiene fragments are in *syn* position if both five-membered rings are attached to vertices of the same color of the parent benzenoid system. Two cyclopentadiene fragments are in *anti* position, if the two five-membered rings are attached to vertices of different color of the parent benzenoid system. For an illustrative example see Fig. 2.

In an earlier work [7] we demonstrated the validity of:

**Theorem 3.** *If $B$ is a Kekuléan benzenoid system, and $D$ is its syn-dicyclopenta derivative, then $n_+(D) = n_-(D)$ and $n_0(D)$, i. e., $D$ has equal number of bonding and antibonding MOs, and has no non-bonding MO.*

In view of this result, in what follows we will consider only *anti*-dicyclopenta derivatives. Let $D$ be such a molecular graph, and let its vertices, edges, and five-membered rings be labeled as indicated in Fig. 3.
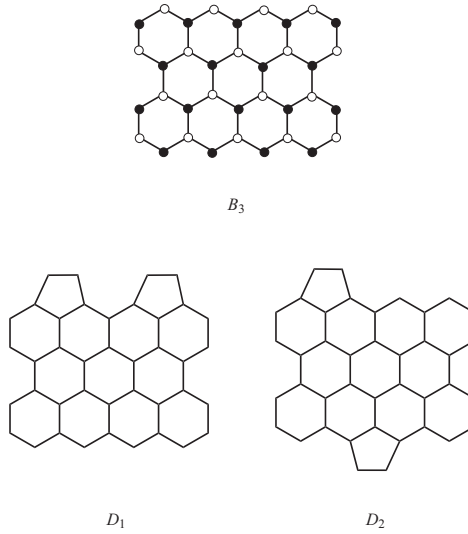
$B_3$



$D_1$                    $D_2$

**Fig. 2.** The parent benzenoid system $B_3$ with its vertices colored, and its two dicyclopenta–derivatives: $D_1$ is a *syn–* and $D_2$ an *anti*-derivative.
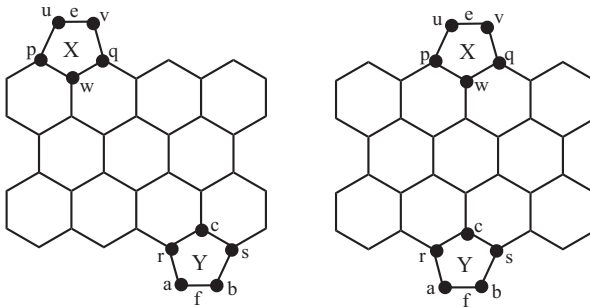


**Fig. 3.** Two *anti*-dicyclopenta-derivatives of a benzenoid system (of $B_3$ from Fig. 2), and the labeling of some of their vertices, edges, and cycles.

Applying Eq. (2) first to the edge $e$ and then to the edge $f$ of $D$ we obtain:

$$\phi(D, \lambda) = \left[ \phi(D - e - f, \lambda) - \phi(D - e - a - b, \lambda) - 2 \sum_Y \phi(D - e - Z_Y, \lambda) \right]$$

$$- \left[ \phi(D - u - v - f, \lambda) - \phi(D - u - v - a - b, \lambda) - 2 \sum_Y \phi(D - u - v - Z_Y, \lambda) \right]$$

$$- 2 \sum_X \left[ \phi(D - Z_X - f, \lambda) - \phi(D - Z_X - a - b, \lambda) - 2 \sum_Y \phi(D - Z_X - Z_Y, \lambda) \right]$$

$$- 2 \sum_{XY} \phi(D - Z_{XY}, \lambda) . \tag{6}$$

In the above formula, $\sum_X$, $\sum_Y$, and $\sum_{XY}$ indicate summation over cycles that, respectively, embrace the ring $X$ but not the ring $Y$, embrace the ring $Y$ but not the ring $X$, and embrace both rings $X$ and $Y$.

First of all, it should be noted that all subgraphs occurring on the right–hand side of Eq. (6) are bipartite and that to all of them the Dewar–Longuet–Higgins formula (5) applies [17]. Some of these have non-zero color excess: $CE(D - e - a - b) = 2$, $CD(D - e - Z_Y) = 1$, $CD(D - u - v - f) = 2$, $CD(D - u - v - Z_Y) = 1$, $CD(D - Z_X - f) = 1$, $CD(D - Z_X - a - b) = 1$. Therefore, by setting $\lambda = 0$ and bearing in mind Lemma 2, we get

$$\phi(D, 0) = \phi(D - e - f, 0) + \phi(D - u - v - a - b, 0)$$

$$+ 4 \sum_X \sum_Y \phi(D - Z_X - Z_Y, 0) - 2 \sum_{XY} \phi(D - Z_{XY}, 0) .$$

Noting that if the parent benzenoid system $B$ has $n$ vertices, then $D$ has $n+4$ vertices, and applying Eq. (5), we have

$$\phi(D, 0) = (-1)^{(n+4)/2} K(D - e - f)^2 + (-1)^{n/2} K(D - u - v - a - b)^2$$

$$+ 4 \sum_X \sum_Y (-1)^{(n+4-|Z_X|-|Z_Y|)/2} K(D - Z_X - Z_Y)^2$$

$$- 2 \sum_{XY} (-1)^{(n+4-|Z_{XY}|)/2} K(D - Z_{XY})^2$$

which immediately yields

$$
\begin{aligned}
(-1)^{(n+4)/2}\,\phi(D,0) \;=\;& K(D-e-f)^2 + K(D-u-v-a-b)^2 \\
&+\; 4\sum_{X}\sum_{Y}(-1)^{(|Z_X|+|Z_Y|)/2}\,K(D-Z_X-Z_Y)^2 \\
&-\; 2\sum_{XY}(-1)^{|Z_{XY}|/2}\,K(D-Z_{XY})^2 \; . \tag{7}
\end{aligned}
$$

From Fig. 3 we see that the subgraph $D-u-v-a-b$ is just the parent benzenoid system $B$. Since by deleting a pendent vertex and its neighbor, the Kekulé structure count does not change [16], the subgraphs $D-e-f$ and $B-p-q-r-s$ have equal $K$-values. Bearing this in mind, Eq. (7) can be rewritten as

$$
\begin{aligned}
(-1)^{(n+4)/2}\,\phi(D,0) \;=\;& K(B)^2 + K(B-p-q-r-s)^2 \\
&+\; 4\sum_{X}\sum_{Y}(-1)^{(|Z_X|+|Z_Y|)/2}\,K(D-Z_X-Z_Y)^2 \\
&-\; 2\sum_{XY}(-1)^{|Z_{XY}|/2}\,K(D-Z_{XY})^2 \; . \tag{8}
\end{aligned}
$$

In what follows we prove that the terms $K(D-Z_X-Z_Y)$ are non-zero only if $|Z_X|+|Z_Y| \equiv 2\;(mod\;4)$ and that the terms $K(D-Z_{XY})$ are non-zero only if $|Z_{XY}| \equiv 0\;(mod\;4)$. If so, then

$$
\begin{aligned}
(-1)^{(n+4)/2}\,\phi(D,0) \;=\;& K(B)^2 + K(B-p-q-r-s)^2 \\
&-\; 4\sum_{X}\sum_{Y}K(D-Z_X-Z_Y)^2 - 2\sum_{XY}K(D-Z_{XY})^2 \; . \tag{9}
\end{aligned}
$$

Then by Lemma 1 we arrive at the conclusion that inequality (1) is a sufficient condition for $n_+(D) \neq n_-(D)$.

What remains to prove are:

**Theorem 4.** *Using the notation specified in Fig. 3, let $Z_X$ and $Z_Y$ be disjoint cycles embracing, respectively, the five-membered cycle $X$ and $Y$. Then the subgraph $D-Z_X-Z_Y$ is Kekuléan (i. e., $K(D-Z_X-Z_Y) > 0$) only if $|Z_X|+|Z_Y| \equiv 2\;(mod\;4)$.*

and

**Theorem 5.** *Using the notation specified in Fig. 3, let $Z_{XY}$ be a cycle embracing both five-membered cycles $X$ and $Y$. Then the subgraph $D - Z_{XY}$ is Kekuléan (i. e., $K(D - Z_{AB} > 0)$ only if $|Z_{XY}| \equiv 0 \ (mod \ 4)$.*

## PROOF OF THEOREM 4

Throughout this section it is assumed that $D$ is a molecular graph of an *anti-dicyclopenta–derivative* of a Kekuléan benzenoid system $B$, and that its vertices and cycles are labeled as indicated in Fig. 3.

We first recall a result valid for benzenoid systems.

**Lemma 6.** [18] *Let $B$ be a benzenoid system and $Z$ its cycle of size $|Z|$. If $|Z| \equiv 0 \ (mod \ 4)$, then inside $Z$ there is an odd number of vertices. If $|Z| \equiv 2 \ (mod \ 4)$, then the number of vertices inside $Z$ is either even or zero.*

We examine the conditions necessary for the validity of $K(D - Z_X - Z_Y) > 0$. As explained above, $K(D - Z_X - Z_Y) > 0$ holds if and only if $D - Z_X - Z_Y$ has no zeros in its spectrum, i. e., $n_0(D - Z_X - Z_Y) = 0$.

The vertices of the subgraph $D - Z_X - Z_Y$ form three disconnected components $D_\alpha$, $D_\beta$, $D_\gamma$ (of which some may be empty). The components $D_\alpha$ and $D_\beta$ are formed by the vertices lying inside the cycles $Z_X$ and $Z_Y$, respectively. The component $D_\gamma$ is formed by the vertices lying outside $Z_Y$ and $Z_Y$. Then

$$K(D - Z_X - Z_Y) = K(D_\alpha) \cdot K(D_\beta) \cdot K(D_\gamma)$$

where, if some of these components is empty (without any vertex), then the respective $K$-value is equal to unity.

The components $D_\alpha, D_\beta, D_\gamma$ are bipartite graphs. If any of them has an odd number of vertices, then its color excess is greater than unity and therefore its $K$-value is equal to zero. Then also $K(D - Z_X - Z_Y) = 0$.

Thus, in order that $K(D - Z_X - Z_Y) > 0$ holds, the number of vertices in all three components $D_\alpha, D_\beta, D_\gamma$ must be even (or zero).

Let $Z$ be a cycle of a graph embedded in the plane. Denote by $n_i(Z)$ the number of vertices lying inside $Z$.

Consider first the case when $Z_X$ is just the five-membered cycle $X$, $|Z_X| = 5$. Inside it there are no vertices, $n_i(Z_X) = 0$, and $|Z_X| \equiv 1 \ (mod \ 4)$.

Consider now the cycles of $D$ that embrace the five-membered cycle $X$, but are greater than $X$. These cycles are of two kinds: those containing the vertex $w$ (for example, $Z_{Xa}$) and those not containing the vertex $w$ (for example, $Z_{Xb}$), cf. Fig. 4.
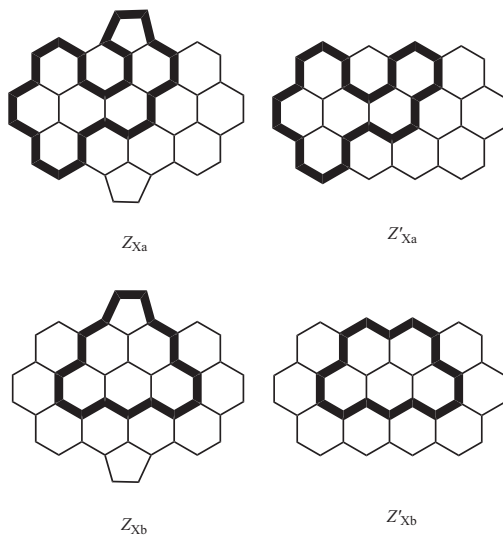


$Z_{Xa}$  $Z'_{Xa}$

$Z_{Xb}$  $Z'_{Xb}$

**Fig. 4.** Two types of cycles ($Z_{Xa}$ and $Z_{Xb}$) in the molecular graphs of *anti*-dicylopenta–derivatives of benzenoid molecules, embracing the five-membered cycle $X$, and the corresponding cycles of the parent benzenoid systems ($Z'_{Xa}$ and $Z'_{Xb}$). In these examples the number of vertices lying inside $Z_{Xa}$ and $Z_{Xb}$ is even, consistent with the fact that $|Z_{Xa}| = 25 = 4 \times 6 + 1$ and $|Z_{Xb}| = 17 = 4 \times 4 + 1$. For details see text.

Let $Z_{Xa}$ be a cycle of $D$, embracing $X$ and containing the vertex $w$, cf. Figs. 3 and 4. This cycle is in a one-to-one correspondence with the cycle $Z'_{Xa}$ of the parent benzenoid system $B$. By inspecting Fig. 4 we see that $n_i(Z_{Xa}) = n_i(Z'_{Xa})$ and $|Z_{Xa}| = |Z'_{Xa}| + 3$. Thus, in order that $n_i(Z_{Xa})$ be even, also $n_i(Z'_{Xa})$ must be even. Then by Lemma 6, $|Z'_{Xa}| \equiv 2 \ (mod \ 4)$ which implies that $|Z_{Xa}| \equiv 1 \ (mod \ 4)$.

Let $Z_{Xb}$ be a cycle of $D$, embracing $X$ but not containing the vertex $w$, cf. Figs.

3 and 4. This cycle is in a one-to-one correspondence with the cycle $Z'_{Xb}$ of the parent benzenoid system $B$. By inspecting Fig. 4 we see that $n_i(Z_{Xb}) = n_i(Z'_{Xb}) + 1$ and $|Z_{Xb}| = |Z'_{Xb}| + 1$. Thus, in order that $n_i(Z_{Xb})$ be even, $n_i(Z'_{Xb})$ must be odd. Then by Lemma 6, $|Z'_{Xb}| \equiv 0 \ (mod \ 4)$ which implies that $|Z_{Xb}| \equiv 1 \ (mod \ 4)$.

Thus is all cases, if the number of vertices inside the cycle $Z_X$ is even (or zero), then $|Z_X| \equiv 1 \ (mod \ 4)$.

By symmetry, the same holds for the cycles $Z_Y$, embracing the five-membered cycle $Y$. From $|Z_X| \equiv 1 \ (mod \ 4)$ and $|Z_Y| \equiv 1 \ (mod \ 4)$ it follows

$$|Z_X| + |Z_Y| \equiv 2 \ (mod \ 4)$$

which is just the claim of Theorem 4. ∎

## PROOF OF THEOREM 5

The proof of Theorem 5 is similar as that of Theorem 4. This time we have to distinguish between four types of cycles in $D$ that embrace both $X$ and $Y$: those containing both vertex $w$ and $c$ (for example, $Z_{XYa}$), those containing the vertex $w$ but not $c$ (for example, $Z_{XYb}$), those containing the vertex $c$ but not $w$ (for example, $Z_{XYc}$), and those containing neither $w$ nor $c$ (for example, $Z_{XYd}$), cf. Figs. 3 and 5

Let $Z_{XYa}$ be a cycle of $D$, embracing $X$ and $Y$ and containing the vertices $w$ and $c$, cf. Figs. 3 and 5. This cycle is in a one-to-one correspondence with the cycle $Z'_{XYa}$ of the parent benzenoid system $B$. By inspecting Fig. 4 we see that $n_i(Z_{XYa}) = n_i(Z'_{XYa})$ and $|Z_{XYa}| = |Z'_{XYa}| + 6$. Thus, in order that $n_i(Z_{XYa})$ be even, also $n_i(Z'_{XYa})$ must be even. Then by Lemma 6, $|Z'_{XYa}| \equiv 2 \ (mod \ 4)$ which implies that $|Z_{XYa}| \equiv 0 \ (mod \ 4)$.

The considerations of the remaining three cases are fully analogous and will be skipped. The final conclusion is that in all cases, if the number of vertices inside the cycle $Z_{XY}$ is even (or zero), then $|Z_{XY}| \equiv 0 \ (mod \ 4)$, which is just the claim of Theorem 5. ∎
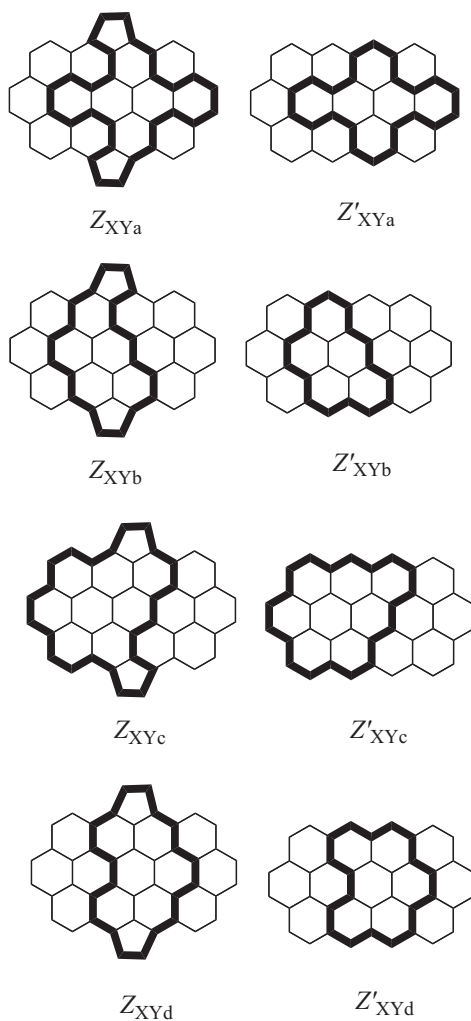
**Fig. 5.** Four types of cycles ($Z_{XYa}$, $Z_{XYb}$, $Z_{XYc}$, and $Z_{XYd}$) in the molecular graphs of *anti*-dicylopenta–derivatives of benzenoid molecules, embracing both five-membered cycles $X$ and $Y$, and the corresponding cycles of the parent benzenoid systems ($Z'_{XYa}$, $Z'_{XYb}$, $Z'_{XYc}$, and $Z'_{XYd}$). In these examples the number of vertices lying inside $Z_{XYa}$, $Z_{XYb}$, $Z_{XYc}$, and $Z_{XYd}$ is even, consistent with the fact that $|Z_{XYa}| = 28 = 4 \times 7$, $|Z_{XYb}| = 20 = 4 \times 5$, $|Z_{XYc}| = 24 = 4 \times 6$, and $|Z_{XYd}| = 20 = 4 \times 5$, For details see text.

## CONCLUDING REMARKS

By means of Theorems 4 and 5 we arrive at Eq. (9), which combined by Lemma 1 results in:

**Theorem 7.** *If B is a Kekuléan benzenoid system, and D is its anti-dicyclopenta derivative, then $n_+(D) \neq n_-(D)$ holds whenever inequality (1) is obeyed.*

From the considerations outlined in the present work, we are not able to decide whether $n_+(D) > n_-(D)$ or $n_+(D) < n_-(D)$ would occur in the case when inequality (1) is satisfied. However, earlier empirical studies [19] clearly point towards the first of the above two options. Thus, we claim [7] that if inequality (1) is satisfied, then the the polycyclic conjugated molecules specified in Theorem 7 have more bonding MOs than antibonding MOs.

A mathematical proof of the latter assertion would be welcome.

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