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A NOTE ON THE RELATIONS BETWEEN THE PERMANENTAL AND CHARACTERISTIC POLYNOMIALS OF CORONOID HYDROCARBONS

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Abstract: A coronoid system is a benzenoid system with a hole, i.e., a non-hexagonal internal face. Several relations between the coefficients of the permanental and characteristic polynomials of benzenoid hydrocarbons were recently established [1]. In this note we investigate relations between the coefficients of the permanental and characteristic polynomials of coronoid hydrocarbons.

INTRODUCTION

The adjacency matrix , $A = (a_{ij})$, of a chemical graph G of n vertices is a matrix of order n consisting of $0's$ and $1's$; where $a_{ij} = 1$ if vertices i and j are adjacent, and $a_{ij} = 0$ otherwise. The characteristic polynomial of the chemical graph G is, by definition [2-4]

$$\phi(G) = \phi(G, \lambda) = det(\lambda I - A) \tag{1}$$

where I is the unit matrix of order n.
The characteristic polynomial can be expressed in coefficient form

$$\phi(G, \lambda) = \sum_{k=0}^{n} a_k \lambda^{n-k} \tag{2}$$

The permanental polynomial is similarly defined as

$$\pi(G) = \pi(G, \lambda) = per(\lambda I - A) \tag{3}$$

and, in parallel to Eq.(2), we write the permanental polynomial in the coefficient form

$$\pi(G,\lambda) = \sum_{k=0}^{n} b_k \lambda^{n-k} \tag{4}$$

In earlier computer-aided studies, several relations between the coefficients of the permanental and characteristic polynomials of benzenoid hydrocarbons and fullerenes were observed [5-6]. The general validity of these empirically discovered regularities were demonstrated in [1].
A coronoid system [7-8] is a benzenoid system with a "hole" which consists of at least two hexagons. A coronoid system G and the benzenoid system B from which G is obtained are depicted in Fig.1. Coronoid systems are the graph representations of the skeletons of coronoid hydrocarbons as well as benzneoid systems are the graph representations of the skeletons of benzenoid hydrocarbons.

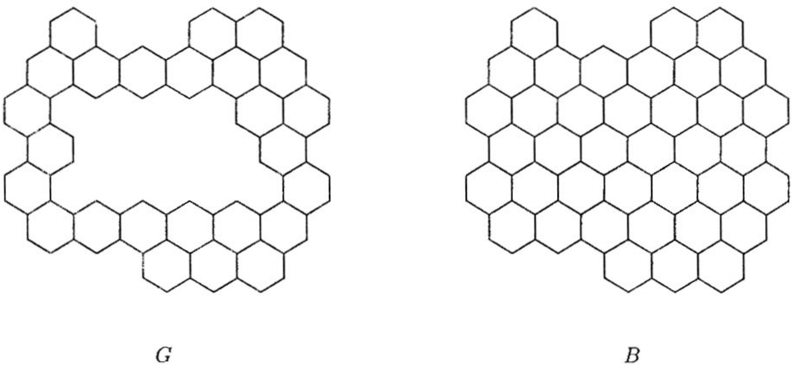

Fig. 1 A coronoid system G and the corresponding benzenoid system B.

In this note we establish some relations between the coefficients of the permanental and characteristic polynomials of coronoid hydrocarbons.

PRELIMINARIES

A Sachs graph S in a molecular graph G is a subgraph of G in which all components are isolated edges and /or cycles containing at least three vertices. By means of the well-known Sachs theorem [9] the coefficients a_k and b_k can be computed from the structure of the molecular graph G. Let $P(S)$ be the number of components of the Sachs graph S in G, and $c(S)$ the number of its cyclic components. Then one has [1,10]

$$a_k = \sum_{s} (-1)^{p(s)} 2^{c(s)} \tag{5}$$

$$b_k = (-1)^k \sum_s 2^{c(s)} \tag{6}$$

Note that the molecular graphs of benzenoid hydrocarbons and coronoid hydrocarbons are bipartite graphs. A bipartite graph possesses no odd-membered cycles, thus no Sachs graphs with odd vertices exist in molecular graphs. Consequently, all odd coefficients in both $\phi(G)$ and $\pi(G)$ are equal to zero. Furthermore, the even coefficients of $\phi(G)$ alternate in sign, whereas all even coefficients of $\pi(G)$ are non-negative:

$$(-1)^k a_{2k} \geq 0; \qquad b_{2k} \geq 0 \qquad \text{for all} \quad k \geq 0.$$

A cycle contained in the molecular graph G is said to be a $(4l)-$cycle if its size is $4l$ for some integer l; i.e., it contains $4l$ vertices. A $(4l+2)-$cycle can be defined in a similar way. By comparing the right-hand sides of Eqs.(5) and (6), one can see that $a_{2k} = (-1)^k b_{2k}$ holds provided the numbers of the components of all $(2k)$-vertex Sachs graphs of G have the same parity. If there exists a $(4l)$-cycle C in G, then there are two $(4l)$-vertex Sachs graphs, say S_1 and S_2 , where S_1 is just the $(4l)-$cycle C ($P(S_1) = 1$, an odd number); whereas S_2 instead of the $(4l)$-cycle has the $2l$ isolated edges contained in C ($P(S_2) = 2l$, an even number). Thus S_1 and S_2 contribute with opposite signs in formula (5) and they subtract from each other; whereas in formula (6) S_1 and S_2 contribute with the same sign and they add. Therefore, $a_{4l} < b_{4l}$ (Note that both a_{4l} and b_{4l} have the same sign: positive).

Lemma 1 Let G be a benzenoid or coronoid system. If q is the size of its shortest $(4l)$-cycle, then $k = q/2$ is the smallest value for which inequality $(-1)^k a_{2k} < b_{2k}$ holds, i.e. :

$$a_{2k} = (-1)^k b_{2k} \quad \text{for} \quad k = 0, 1, 2, \cdots, q/2 - 1; \tag{7}$$

and

$$a_q < b_q \tag{8}$$

Proof. As mentioned above, if G possesses a $(4l)$-cycle with $4l = q$, we have $a_{4l} < b_{4l}$, i.e., $a_q < b_q$. Now we prove that Eq. 7 holds. As q is the size of its shortest $(4l)$-cycle, there is no $(4l)$-cycle for $4l < q$. Let S^* be a $2k$-vertex Sachs graph, where $2k < q$. Suppose that S^* possesses u cycles and v isolated edges, i.e., the number of components of S^* is $u + v$. The size of these cycles are $4l_1 + 2, 4l_2 + 2, 4l_3 + 2, \cdots, 4l_u + 2$. Then $2k = 4(l_1 + l_2 + \cdots + l_u) + 2u + 2v$. Therefore, $u + v = k - 2(l_1 + l_2 + \cdots + l_u)$, which means that the number of the components of S^* has the same parity as that of k. In other words, all $2k$-vertex Sachs graphs with $2k < q$ have either even or odd number of components. Consequently, Eq. 7 holds.

Lemma 2 Let G be a benzenoid or coronoid system. If k^* is the smallest value for which inequality $(-1)^k a_{2k} < b_{2k}$ holds, then $q = 2k^*$ is the size of the shortest $(4l)$-cycle in G.

Proof. Since $(-1)^k a_{2k} = b_{2k}$ for $k < k^*$, there is no $(4l)$-cycle in G with $4l < 2k^*$. Now we prove that there is a $(4l)$-cycle in G with $4l = 2k^*$, namely, $q = 2k^*$ is the size of the shortest $(4l)$-cycle in G. By contradiction. If there is no $(4l)$-cycle in G with $4l = 2k^*$, then as mentioned in the proof of Lemma 1, $(-1)^k a_{2k^*} = b_{2k^*}$, contradicting that k^* satisfies the inequality $(-1)^k a_{2k} < b_{2k}$.

As a direct consequence of the above two lemmas, we have:

Lemma 3 Let G be a benzenoid or coronoid system. Then positive integer k is the smallest value for which the inequality $(-1)^k a_{2k} < b_{2k}$ holds if and only if positive integer $q = 2k$ is the size of the shortest $(4l)$-cycle in G.

The known results about the relations between the coefficients of the characteristic and permanental polynomials are as follows:

Theorem 4[1] If G is the molecular graph of a cata-condensed benzenoid hydrocarbon, then the following property holds:

$$\text{Property}^* : a_{2k} = (-1)^k b_{2k} \quad \text{for} \quad \text{all} \quad k = 0, 1, 2, \cdots.$$

Theorem 5[1] If G is the molecular graph of a planar peri-condensed benzenoid hydrocarbon, then $a_{2k} = (-1)^k b_{2k}$ for $k = 0, 1, 2, 3, 4, 5$; and $a_{12} = b_{12} - 4n_i$, where n_i is the number of internal vertices of G.

PERI-CONDENSED CORONOID HYDROCARBONS

From now on we confine ourselves to coronoid systems. Let G be a coronoid system. By C_i and C_o we denote the inner and the outer perimeters of G, respectively. The size of C_i and C_o are denoted by $|C_i|$ and $|C_o|$, respectively. For planar peri-condensed coronoid systems (i.e. coronoid systems possessing internal vertices), we have the following.

Theorem 6 If G is the molecular graph of a planar peri-condensed coronoid hydrocarbon, then $a_{2k} = (-1)^k b_{2k}$ for $k = 0, 1, 2, 3, 4, 5$; and $a_{12} = b_{12} - 4(n_i + t)$, where n_i is the number of internal vertices of G and t is determined by

$$t = \begin{cases} 0, & \text{if } |C_i| > 12 \\ 1, & \text{if } |C_i| = 12 \\ 2, & \text{if } |C_i| = 10 \end{cases}$$

Proof. It is clear that each internal vertex in G corresponds to a 12-cycle which is the shortest $(4l)$-cycle in G. By Lemma 1, $a_{2k} = (-1)^k b_{2k}$ for $k = 0, 1, 2, 3, 4, 5$; and $a_{12} < b_{12}$. If $|C_i| > 12$, there are exactly n_i 12-cycles in G. Hence $a_{12} = b_{12} - 4n_i$. If C_i is itself a 12-cycle, there are $(n_i + 1)$ 12-cycles in G and thus $a_{12} = b_{12} - 4(n_i + 1)$. In the case C_i is a 10-cycle, there are two additional 12-cycles which do not depend on any internal vertex of G (cf. Fig.2). Therefore, $a_{12} = b_{12} - 4(n_i + 2)$.

Fig. 2 A peri-condensed coronoid system G with two 12−cycles which do not depend on any internal vertex of G.

CATA-CONDENSED CORONOID HYDROCARBONS

Cata-condensed coronoid systems are also called primitive coronoids [7]. To our surprise, the situation for cata-condensed coronoid systems is much more complicated than that of cata-condensed benzenoid systems. Unlike cata-condensed benzenoid systems, there is no cata-condensed coronoid system satisfying Property *: $a_{2k} = (-1)^k b_{2k}$ for all $k = 0, 1, 2, \cdots$.

Let G be a coronoid system. Recall that the dual graph [11] $D(G)$ of G is a graph in which each vertex corresponds to one hexagon of G, and two vertices are connected by an edge when the two corresponding hexagons share an edge. A cata-condensed coronoid system G and the corresponding dual graph $D(G)$ are depicted in Fig.3

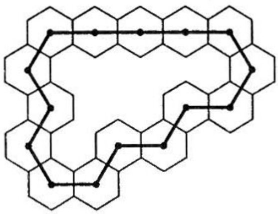

Fig. 3 A cata-condensed coronoid system and the corresponding dual graph.

It is evident that in $D(G)$ there are three different kinds of angles: angles of 120^o, angles of 180^o and angles of 240^o. With the help of dual graphs, some basic properties for cata-condensed coronoid systems are found.

Lemma 7 Let G be a cata-condensed coronoid system. Then we have

1. the number of angles of 120^o in $D(G)$ is larger than that of angles of 240^o in $D(G)$ by six;
2. the size of C_o is larger than that of C_i by twelve, i.e., $|C_o| - |C_i| = 12$;
3. if C_i is a $(4l)$-cycle for some integer l, then C_o is a $(4l')$-cycle for some integer l'; moreover, if C_i is a $(4l+2)$-cycle for some integer l, then C_o is a $(4l'+2)$-cycle for some integer l'.

Proof. Suppose that the numbers of angles of $120^o, 240^o$ and 180^o in $D(G)$ are x, y and z, respectively. If we disregard the angles of 180^o, then by the inner-angle-sum rule for polygons in geometry, we have:

$$120^o \times x + 240^o \times y = 180^o \times (x + y - 2)$$

Therefore,

$$x - y = 6, \tag{9}$$

which means that the number of angles of 120^o is larger than that of angles of 240^o by six (cf. Fig. 3).

It is not difficult to see that a hexagon of G contributes one, two and three edges, respectively, to C_i if its corresponding angle in $D(G)$ is an angle of $120^o, 180^o$ and 240^o, respectively (cf. Fig.3). Then we have

$$|C_i| = x + 3y + 2z \tag{10}$$

In an analogous way, we reach at

$$|C_o| = 3x + y + 2z \tag{11}$$

Combining Eqs. (10) and (11), one has

$$|C_o| - |C_i| = 2(x - y) \tag{12}$$

Inserting Eq. (9) into Eq(12), we have

$$|C_o| - |C_i| = 2 \times 6 = 12 \tag{13}$$

Now assume that C_i is a $(4l)$-cycle, i.e. $|C_i| = 4l$. Then by Eq. (13), $|C_o| = |C_i| + 12 = 4(l + 3)$, which implies that C_o is a $(4l')$-cycle, where $l' = l + 3$. Similarly, if C_i is a $(4l + 2)$-cycle, then C_o is a $(4l' + 2)$-cycle, where $l' = l + 3$.

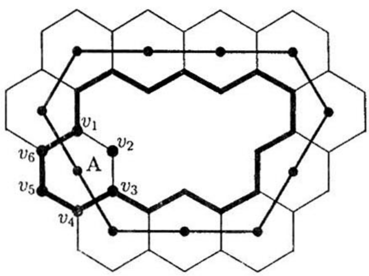

Fig. 4 An illustration for the proof of Lemma 8.

Lemma 8 Let G be a cata-condensed coronoid system. If $D(G)$ possesses an angle of 180^o, then there is a cycle of size $(|C_i| + 2)$ in G.

Proof. Let hexagon A of G correspond to an angle of 180^o in $D(G)$, $v_1, v_2, ..., v_6$ be the six vertices of A . Denote by C^* (marked by heavy lines in Fig. 4) the cycle obtained from C_i by deleting vertex v_2 and adding vertices v_4, v_5 and v_6. Then C^* is a cycle in G of size $|C^*| = |C_i| - 1 + 3 = |C_i| + 2$.

Lemma 9 Let G be a cata-condensed coronoid system. Then there is a cycle of size $(|C_i| + 2)$ in G.

Proof. If there is neither angle of 180^o, nor angle of 240^o in $D(G)$, G is the benzenoid system depicted in Fig. 5, contradicting that G is a coronoid system. Therefore,there is

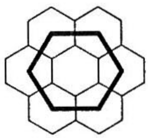

Fig. 5 The only system whose dual graph possesses angles of 120^o only.

at least an angle of 180^o or an angle of 240^o in $D(G)$. If there is an angle of 180^o in $D(G)$, by Lemma 8, there is a cycle with size $(|C_i| + 2)$ in G. Now suppose that there is no angle of 180^o, but at least an angle of 240^o in $D(G)$. As mentioned in Lemma 7, there are more angles of 120^o than angles of 240^o in $D(G)$. Therefore, there are two neighboring angles in $D(G)$ with one being of 120^o and the other being of 240^o. In a similar way, a cycle of size $(|C_i| + 2)$ can be found in G (marked by heavy lines in Fig. 6).

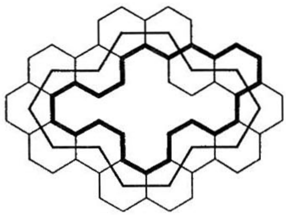

Fig. 6 An illustration for the proof of Lemma 9.

Theorem 10 Let G be a cata-condensed coronoid system. Then G does not satisfy Property *: $a_{2k} = (-1)^k b_{2k}$ for all $k = 0, 1, 2, \cdots$.

Proof. It suffices to prove that there is a $(4l)$-cycle in G. If $|C_i| = 4l$, the inner perimeter C_i is itself a $4l$-cycle, and there is nothing to prove. Now suppose $|C_i| = 4l + 2$. By Lemma 7, $|C_o| = 4l' + 2$. Thus neither C_i nor C_o is a $4l$-cycle, and we need to find a cycle in G of size $4l^*$, which is neither C_i, nor C_o. By Lemma 9, there is a cycle of size $|C_i| + 2 = (4l + 2) + 2 = 4(l + 1)$, which is a $(4l^*)$-cycle with $l^* = l + 1$.

Now a natural question emerges: what is the smallest value of k for which the inequality

$(-1)^k a_{2k} < b_{2k}$ holds? or equally, what is the size of the shortest $(4l)$−cycle? One can check that the two cata-condensed coronoid systems G_1 and G_2 depicted in Fig.7 have the same size of inner perimeter: $|C_i| = 52$, and in each of $D(G_1)$ and $D(G_2)$ there are three angles of 180^o, ten angles of 240^o and sixteen angles of 120^o. But in G_1 the shortest $(4l)$-cycle is a 44-cycle, whereas in G_2 the shortest $(4l)$-cycle is a 52-cycle. This is mainly caused by the way in which the angles of 240^o appear in the sequence of inner angles of $D(G_i)$.

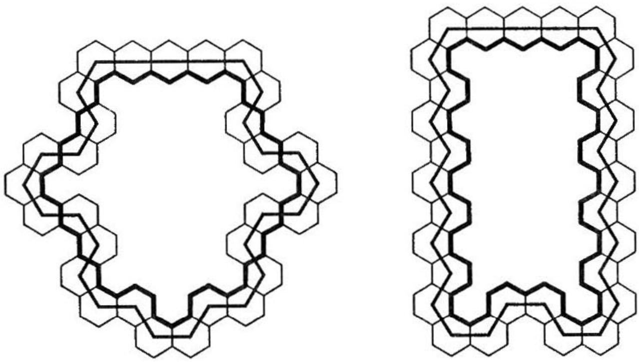

Fig. 7 Two cata-condensed coronoid systems with the same size of inner perimeter, but different size of the shortest $(4l)$-cycles.

Definition 11 Suppose that angles of 180^o are disregarded. Let $a_i, a_{i+1}, \cdots, a_{i+k}, a_{i+k+1}$ be $k+2 (k \geq 2)$ consecutive angles in $D(G)$. If a_i and a_{i+k+1} are angles of 120^o, and all the angles $a_{i+1}, a_{i+2}, \cdots, a_{i+k}$ are angles of 240^o, then $\{a_{i+1}, a_{i+2}, \cdots, a_{i+k}\}$ is said to be a normal set of angles of 240^o of size $k(\geq 2)$ (cf. Fig.8).

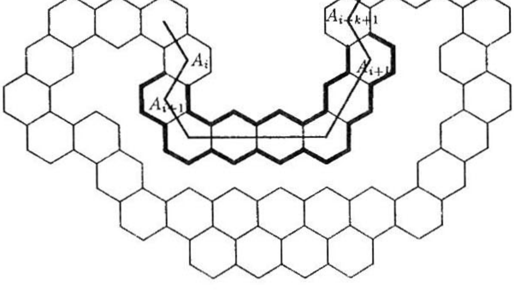

Fig. 8 A normal set of angles of 240^o with size $k = 4$

Lemma 12 Let G be a cata-condensed coronoid system. If $D(G)$ possesses a normal set of angles of 240^o of size k, then there is a cycle in G of size $(|C_i| - 2(k-1))$.

Proof. Suppose that $D(G)$ possesses a normal set of angles of 240^o of size k. Then there is a series of angles $a_i, a_{i+1}, \cdots, a_{i+k}, a_{i+k+1}$ in $D(G)$, where a_i and a_{i+k+1} are angles of 120, and all the angles $a_{i+1}, a_{i+2}, \cdots, a_{i+k}$ are angles of 240^o. Let the corresponding hexagons of G be $A_i, A_{i+1}, \cdots, A_{i+k}$ and A_{i+k+1}. Note that when normal sets of angles of 240^o are mentioned, angles of 180^o are disregarded. Now suppose that there are altogether z angles of 180^o among the angles $a_i, a_{i+1}, \cdots, a_{i+k}$ and a_{i+k+1} (cf. Fig. 8, $z = 3$). Bear in mind that a hexagon of G which corresponds to an angle of 240^o in $D(G)$ contributes three edges to C_i and one edge to C_o, respectively; whereas a hexagon of G contributes two edges to each of C_i and C_o if it corresponds to an angle of 180^o in $D(G)$. Therefore, the size of the segment of C_i between A_{i+1} and A_{i+k} (marked by heavy lines in Fig. 8) equals to $3k + 2z$, whereas the size of the segment of C_o between A_{i+1} and A_{i+k} (cf. Fig. 8) equals to $k + 2z$. Now one can obtain a cycle C^* from C_i by deleting the segment of C_i between A_{i+1} and A_{i+k}; and adding the segment of C_o between A_{i+1} and A_{i+k} and the two edges shared by A_i and A_{i+1}, A_{i+k} and A_{i+k+1}, respectively. It is evident that the size of C^* is $|C^*| = |C_i| - [(3k + 2z) - (k + 2z)] + 2 = |C_i| - 2(k-1)$.

Lemma 13 Let G be a cata-condensed coronoid system. If $D(G)$ possesses a normal set of angles of 240^o of size k, then there is a cycle in G of size $(|C_i| - 2(r-1))$, where $2 \leq r \leq k$.

Proof. Suppose that $\{a_{i+1}, a_{i+2}, \cdots, a_{i+k}\}$ is a normal set of angles of 240^o of size k. Evidently, $\{a_{i+1}, a_{i+2}, \cdots, a_{i+r}(2 \leq r \leq k)\}$ is a subset of $\{a_{i+1}, a_{i+2}, \cdots, a_{i+k}\}$. In an analogous way as in the proof of Lemma 12 (cf. Fig. 9, where $k = 4, r = 3$), there is a cycle in G of size $(|C_i| - 2(r-1))$, where $2 \leq r \leq k$.

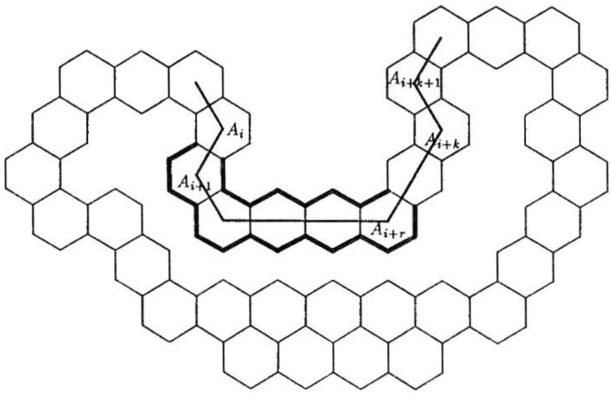

Fig. 9 An illustration for the proof of Lemma 13

Corollary 14 Let G be a cata-condensed coronoid system. If $D(G)$ possesses t normal sets of angles of 240^o, and the corresponding size are $k_1, k_2, \cdots, k_{t-1}, k_t$; then there is a

cycle in G of size r satisfying $(|C_i| - \sum_{i=1}^{t} 2(k_i - 1)) \le r \le (|C_i| - 2)$.
Proof. Directly from lemmas 12 and 13.

It is known that the length of the outer perimeter C_o is larger than that of the inner perimeter C_i by twelve (Lemma 7). Therefore, if we want to search the shortest $(4l)$-cycles in G, it is better to start from C_i. By the above corollary, whether or not we can find a $(4l)$-cycle shorter than C_i in G depends on whether or not there is any normal set of angles of 240^o in $D(G)$. We have the following theorems:

Theorem 15 Let G be a cata-condensed coronoid system. Suppose that $|C_i| = 4u+2$. The size q of the shortest $(4l)$-cycle in G is determined by

$$q = \begin{cases} |C_i| - \sum_{i=1}^{t} 2(k_i - 1), & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l + 2 \\ |C_i| - \sum_{i=1}^{t} 2(k_i - 1) + 2, & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l \\ |C_i| + 2, & \text{if there is no normal set of angles of } 240^o, \end{cases}$$

Theorem 16 Let G be a cata-condensed coronoid system. Suppose that $|C_i| = 4u$. Then the size q of the shortest $(4l)$-cycle in G is is determined by

$$q = \begin{cases} |C_i| - \sum_{i=1}^{t} 2(k_i - 1), & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l \\ |C_i| - \sum_{i=1}^{t} 2(k_i - 1) + 2, & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l + 2 \\ |C_i|, & \text{if there is no normal set of angles of } 240^o \end{cases}$$

The following theorems are the direct corollaries of Lemma 3 and the above two theorems:

Theorem 17 Let G be a cata-condensed coronoid system. Suppose that $|C_i| = 4u+2$. Then

$$a_{2k} = (-1)^k b_{2k} \quad \text{for} \quad k = 0, 1, 2, \cdots, q/2 - 1$$

and

$$a_q < b_q$$

q is determined by

$$q = \begin{cases} |C_i| - \sum_{i=1}^{t} 2(k_i - 1), & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l + 2 \\ |C_i| - \sum_{i=1}^{t} 2(k_i - 1) + 2, & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l \\ |C_i| + 2, & \text{if there is no normal set of angles of } 240^o, \end{cases}$$

Theorem 18 Let G be a cata-condensed coronoid system. Suppose that $|C_i| = 4u$. Then

$$a_{2k} = (-1)^k b_{2k} \quad \text{for} \quad k = 0, 1, 2, \cdots, q/2 - 1$$

and

$$a_q < b_q$$

q is determined by

$$q = \begin{cases} |C_i| - \sum_{i=1}^{t} 2(k_i - 1), & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l \\ |C_i| - \sum_{i=1}^{t} 2(k_i - 1) + 2, & \text{if there are normal sets of angles of } 240^o, \\ & \text{and } \sum_{i=1}^{t} 2(k_i - 1) = 4l + 2 \\ |C_i|, & \text{if there is no normal set of angles of } 240^o \end{cases}$$

REMARK

By Theorems 17 and 18, the smallest value k for which the inequality $(-1)^k a_{2k} < b_{2k}$ holds is known. It is interesting that the difference between b_{2k} and $(-1)^k a_{2k}$ is often very large. This is caused by the fact that the number of the shortest $(4l)$−cycles in G is very large. Let us look at the cata-condensed coronoid system depicted in Fig. 10. The inner perimeter C_i is a 68−cycle, and there is no normal set of angles of 240^o. By Theorem 16, C_i is one of the shortest $(4l)$-cycle in G. One can check that there are 53 different ways for a cycle of G to go through A to B with the same length. Similarly, there are 53 different ways for a cycle of G to go through C to D with the same length . Consequently, there are at least $53 \times 53 = 2809$ different 68-cycles in G.

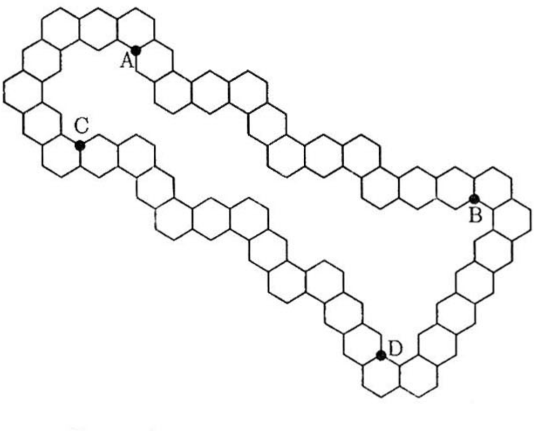

Fig. 10 A cata-condensed coronoid system

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