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The extremal pentagon-chain polymers with respect to permanental sum

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The permanental sum of a graph *G* can be defined as the sum of absolute value of coefficients of permanental polynomial of *G*. It is closely related to stability of structure of a graph, and its computing complexity is #P-complete. Pentagon-chain polymers is an important type of organic polymers. In this paper, we determine the upper and lower bounds of permanental sum of pentagon-chain polymers, and the corresponding pentagon-chain polymers are also determined.

The *permanent* of an $n \times n$ real matrix $M = (m_{ij})$, with $i, j \in \{1, 2, \ldots, n\}$, is defined as

$$\mathrm{per}(M) = \sum_{\sigma} \prod_{i=1}^{n} m_{i\sigma(i)},$$

where the sum is taken over all permutations σ of $\{1, 2, \ldots, n\}$.

Let $A(G)$ be an adjacency matrix of a graph G of order n with a given vertex labeling. The *permanental polynomial* of G is defined as

$$\pi(G, x) = \mathrm{per}(xI - A(G)) = \sum_{k=0}^{n} b_k(G) x^{n-k}$$

with $b_0(G) = 1$.

Earlier, Kasum et al.[1] and Merris et al.[2] give a graphical interpretation of the coefficients of the permanental polynomial of G using linear subgraphs: for $1 \leq k \leq n$,

$$b_k(G) = (-1)^k \sum_{H \in S_k(G)} 2^{c(H)},$$

where $S_k(G)$ is the collection of all linear subgraphs H of order k in G, and $c(H)$ is the number of cycles in H. Recall that A *linear subgraph* of a graph G is termed as a subgraph whose components are cycles or single edges.

The *permanental sum* of G, denoted by $PS(G)$, is the sum of the absolute values of all coefficients of $\pi(G, x)$, i.e.,

$$PS(G) = \sum_{k=0}^{n} |b_k(G)| = 1 + \sum_{k=1}^{n} \sum_{H \in S_k(G)} 2^{c(H)}.$$

Background. The study of permanental polynomial of a graph in chemical literature were started by Kasum et al.[1]. They computed respectively permanental polynomials of paths and cycles, and zeroes of these polynomials. Cash[3] investigated permanental polynomials of some chemical graphs(including benzene, *o*-biphenylene, coronene, C_{20} fullerene). And he pointed out that studying the absolute values of coefficients of permanental polynomials is of interest. However, it is difficult to compute the coefficients of permanental polynomial of a graph. Up to now, only a few about the coefficients of permanental polynomials of chemical graphs and its potential applications seems to have been published[4–14]. A natural problem is researching the sum of coefficients of permanental polynomials of a chemical graph, i.e., how characterize the permanental sum of a chemical graph. There exists a peculiar chemical phenomenon which closely relate to the permanental sum. For the theo-

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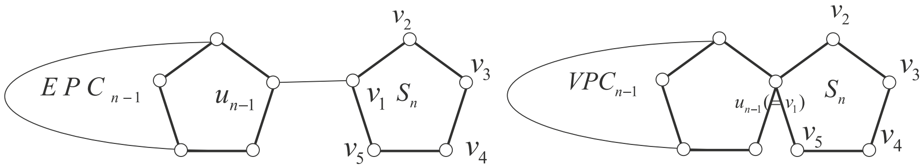

Figure 1. An edge-pentagon-chain EPC_n and a vertex-pentagon-chain VPC_n.

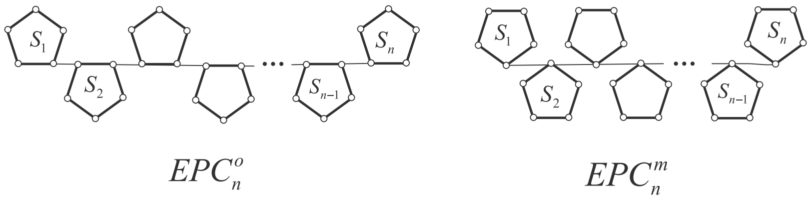

Figure 2. An edge-ortho-pentagon-chain EPC_n^o and an edge-meta-pentagon-chain EPC_n^m.

retical study of nature, there exists 271 nonisomorphic fullerenes in C_{50}. Up to now, only a few fullerenes in C_{50} is found. In 2004, Xie et al.[15] captured a labile fullerene $C_{50}(D_{5h})$. Tong et al.[16] computed the permanental sums of all 271 fullerenes in C_{50}. They found that the permanental sum of $C_{50}(D_{5h})$ achieves the minimum among all 271 fullerenes in C_{50}, and they also pointed out that the permanental sum could be closely related to the stability of molecular graphs. A bad news is the computing complexity of permanental sum is #P-complete[17]. In spite of this difficulty, the studies of permanental sums have received a lot of attention from researchers in recent years. Chou et al.[18] studied the property of C_{70}. Li et al.[19] determined the extremal hexagonal chains with respect to permanental sum. Li and Wei[20] characterized the extremal octagonal chains with respect to permanental sum. Wu and Lai[21] study some basic properties of the permanental sum of general graphs, in particular, they pointed out that the permanental sum is closed to the Fibonacci numbers. For the background and some known results about this problem, we refer the reader to[22–25] and the references therein.

In addition, the permanental sum is similar to Hosoya index proposed by Haruo Hosoya. *Hosoya index* of a graph G, denoted by $Z(G)$, is defined as the total number of independent edge sets of G[26]. The Hosoya index is closely related to the boiling points of chemical graphs. Wu and Lai[21] shown that $PS(G) \geq Z(G)$ with the equality holds if and only if G is a forest. These indicate that the permanental sum is likely to explain certain characteristics of chemical molecules.

Base on arguments as above, it is interesting to study the permanental sums of chemical graphs.

The graph model of a type of organic polymers. Organic polymers are a fascinating class of chemical materials with a strikingly wide range of applications[27–32]. Many of them contain chains of five-membered rings as a building block, see Figure 1 in[33]. It is easy to see that the graph model of the organic polymer with n five-membered rings is an edge-pentagon-chain. An *edge-pentagon-chain* EPC_n with n pentagons, which is a sub-chain of an edge-pentagon-chain, can be regarded as an edge-pentagon-chain EPC_{n-1} with $n-1$ pentagons adjoining to a new terminal pentagon by a cut edge, see Fig. 1. By contracting operation of graphs, an edge-pentagon-chain EPC_n with n pentagons is changed new pentagon-chain called *vertex-pentagon-chain*. That is, A *vertex-pentagon-chain*, denoted by VPC_n, is obtained by contracting every cut edge in EPC_n, see Fig. 1. Checking the structure of a vertex-pentagon-chain, it is not difficult to see that the vertex-pentagon-chain also is a graph model of a type of organic polymers[34,35].

In this paper, we focus on properties of permanental sum of pentagon-chain polymers. We hope that results of the paper will provide theoretical support for the study of organic polymers.

Preliminaries. Let $EPC_n = S_1S_2\cdots S_n$ be a polyomino chain with $n(\geq 2)$ pentagons, where S_k is the k-th pentagon in EPC_n attached to S_{k-1} by a cut edge $u_{k-1}w_k$, $k = 2, 3, \ldots, n$, where $w_k = v_1$ is a vertex of S_k. A vertex v is said to be *ortho*- and *meta*-vertex of S_k if the distance between v and w_k is 1 and 2, denoted by o_k and m_k, respectively. Checking Fig. 1, it is easy to see that $w_n = v_1$, ortho-vertices $o_n = v_2, v_5$, and meta-vertex $m_n = v_3, v_4$ in S_n.

An edge-pentagon-chain EPC_n is an *edge-ortho-pentagon-chain* if $u_k = o_k$ for $2 \leq k \leq n-1$, denoted by EPC_n^o. An edge-pentagon-chain EPC_n is an *edge-meta-pentagon-chain* if $u_k = m_k$ for $2 \leq k \leq n-1$, denoted by EPC_n^m. The resulting graphs see Fig. 2. Contracting every cut edge in EPC_n^o and EPC_n^m, the resulting graphs are called a *vertex-ortho-pentagon-chain* VPC_n^o and a *vertex-meta-pentagon-chain* VPC_n^m, respectively. See Fig. 3.

In[21], some properties of permanental sum of a graph are determined.

Lemma 1.1 [21] *Let P_n be a path with n vertices. Then*

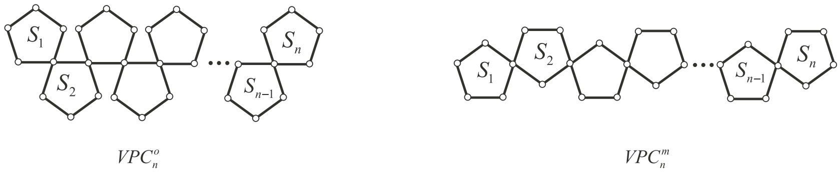

Figure 3. A vertex-ortho-pentagon-chain VPC_n^o and a vertex-meta-pentagon-chain VPC_n^m.

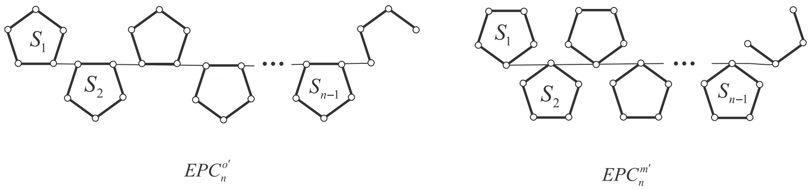

Figure 4. Chains $EPC_n^{o'}$ and $EPC_n^{m'}$.

$$PS(P_n) = \begin{cases} 1 & \text{if } n = 0, \\ 1 & \text{if } n = 1, \\ F_{n+1} & \text{if } n \geq 2, \end{cases}$$

where $F(0) = 0, F(1) = 1$ *and* $F(n) = F(n-1) + F(n-2)$ *for* $n \geq 2$ *denotes the sequence of Fibonacci numbers.*

Lemma 1.2 [21] *The permanental sum of a graph satisfies the following identities:*
(i) Let G and H be two connected graphs. Then

$$PS(G \cup H) = PS(G)\,PS(H).$$

(ii) Let $e = uv$ *be an edge of a graph G and* $\mathcal{C}(e)$ *the set of cycles containing e. Then*

$$PS(G) = PS(G-e) + PS(G-v-u) + 2\sum_{C_k \in \mathcal{C}(e)} PS(G - V(C_k)).$$

(iii) Let v be a vertex of a graph G and $\mathcal{C}(v)$ *the set of cycles containing v. Then*

$$PS(G) = PS(G-v) + \sum_{u \in N_G(v)} PS(G-v-u) + 2\sum_{C_k \in \mathcal{C}(v)} PS(G - V(C_k)).$$

By Lemma 1.2, we obtain the following corollary.

Corollary 1.1 *Let G be a graph and v a vertex of G. Then* $PS(G-v) < PS(G)$.

Results

The bound of permanental sum of edge-pentagon-chains. In order to prove the lemma 2.1, we give two auxiliary graphs. One is denoted by $EPC_n^{o'}$ obtained from EPC_n^o deleting a ortho-vertex in S_n. The other is denoted by $EPC_n^{m'}$ obtained from EPC_n^m deleting meta-vertex in S_n. The resulting graphs see Fig. 4.

Lemma 2.1 *Let* EPC_n^o *and* EPC_n^m *be an edge-ortho-pentagon-chain and an edge-meta-pentagon-chain, respectively. Then*

$$PS(EPC_n^o) = \frac{194 + 137\sqrt{2}}{2}\left(8 + 5\sqrt{2}\right)^{n-2} + \frac{194 - 137\sqrt{2}}{2}\left(8 - 5\sqrt{2}\right)^{n-2},$$

$$PS(EPC_n^m) = \frac{640237 + 43067\sqrt{221}}{442}\left(\frac{15 + \sqrt{221}}{2}\right)^{n-3} + \frac{640237 - 43067\sqrt{221}}{442}\left(\frac{15 - \sqrt{221}}{2}\right)^{n-3}.$$

Proof By Lemma 1.2, we have

$$PS(EPC_n^o) = 13PS(EPC_{n-1}^o) + 5PS(EPC_{n-1}^{o'}),$$
$$PS(EPC_n^{o'}) = 5PS(EPC_{n-1}^o) + 3PS(EPC_{n-1}^{o'}).$$

Thus,

$$\begin{pmatrix} PS(EPC_n^o) \\ PS(EPC_n^{o'}) \end{pmatrix} = \begin{pmatrix} 13 & 5 \\ 5 & 3 \end{pmatrix} \begin{pmatrix} PS(EPC_{n-1}^o) \\ PS(EPC_{n-1}^{o'}) \end{pmatrix}.$$

Direct computation yields $PS(EPC_2^o) = 194$ and $PS(EPC_2^o) = 80$. Now,

$$\begin{aligned} PS(EPC_n^o) &= 13PS(EPC_{n-1}^o) + 5PS(EPC_{n-1}^{o'}), \\ &= (13\ \ 5) \begin{pmatrix} 13 & 5 \\ 5 & 3 \end{pmatrix} \begin{pmatrix} PS(EPC_{n-2}^o) \\ PS(EPC_{n-2}^{o'}) \end{pmatrix} \\ &= \cdots \\ &= (13\ \ 5) \begin{pmatrix} 13 & 5 \\ 5 & 3 \end{pmatrix}^{n-3} \begin{pmatrix} 194 \\ 80 \end{pmatrix}. \end{aligned} \tag{1}$$

Set matrix $M = \begin{pmatrix} 13 & 5 \\ 5 & 3 \end{pmatrix}$. Then the characteristic polynomial of M equals to $x^2 - 16x + 14$. Solving $x^2 - 16x + 14 = 0$, we obtain that the eigenvalues of M are $8 + 5\sqrt{2}$ and $8 - 5\sqrt{2}$, respectively. And the corresponding eigenvectors of these eigenvalues are $T_1 = \begin{pmatrix} 1 \\ \sqrt{2}-1 \end{pmatrix}$ and $T_2 = \begin{pmatrix} -1 \\ \sqrt{2}+1 \end{pmatrix}$.

Let $T = \begin{pmatrix} 1 & -1 \\ \sqrt{2}-1 & \sqrt{2}+1 \end{pmatrix}$. Then the inverse matrix of T is $T^{-1} = \begin{pmatrix} \frac{\sqrt{2}+2}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}-2}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$. According to the property of a similarity matrix, we have

$$T^{-1}MT = \begin{pmatrix} 8+5\sqrt{2} & 0 \\ 0 & 8-5\sqrt{2} \end{pmatrix}.$$

Therefore,

$$M = T \begin{pmatrix} 8+5\sqrt{2} & 0 \\ 0 & 8-5\sqrt{2} \end{pmatrix} T^{-1}. \tag{2}$$

By (1) and (2), we have

$$\begin{aligned} PS(EPC_n^o) &= (\,13\ \ 5\,) \begin{pmatrix} 1 & -1 \\ \sqrt{2}-1 & \sqrt{2}+1 \end{pmatrix} \begin{pmatrix} 8+5\sqrt{2} & 0 \\ 0 & 8-5\sqrt{2} \end{pmatrix}^{n-3} \begin{pmatrix} \frac{\sqrt{2}+2}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}-2}{4} & \frac{\sqrt{2}}{4} \end{pmatrix} \begin{pmatrix} 194 \\ 80 \end{pmatrix} \\ &= \left(\frac{194 + 137\sqrt{2}}{2} \right) (8+5\sqrt{2})^{n-2} + \left(\frac{194 - 137\sqrt{2}}{2} \right) (8-5\sqrt{2})^{n-2}. \end{aligned}$$

Similarly, by Lemma 1.2, we obtain

$$\begin{aligned} PS(EPC_n^m) &= 13PS(EPC_{n-1}^m) + 5PS(EPC_{n-1}^{m'}), \\ PS(EPC_n^{m'}) &= 5PS(EPC_{n-1}^m) + 2PS(EPC_{n-1}^{m'}). \end{aligned}$$

So,

$$\begin{pmatrix} PS(EPC_n^m) \\ PS(EPC_n^{m'}) \end{pmatrix} = \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix} \begin{pmatrix} PS(EPC_{n-1}^m) \\ PS(EPC_{n-1}^{m'}) \end{pmatrix}.$$

Direct computation yields $PS(EPC_2^m) = 194$ and $PS(EPC_2^m) = 75$. Then,

$$\begin{aligned} PS(EPC_n^m) &= 13PS(EPC_{n-1}^m) + 5PS(EPC_{n-1}^{m'}) \\ &= (13\ \ 5) \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix} \begin{pmatrix} PS(EPC_{n-2}^m) \\ PS(EPC_{n-2}^{m'}) \end{pmatrix} \\ &= \cdots \\ &= (13\ \ 5) \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix}^{n-3} \begin{pmatrix} 194 \\ 75 \end{pmatrix}. \end{aligned} \tag{3}$$

Let $M = \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix}$ be a matrix. Then the eigenvalues of M are $\frac{15+\sqrt{221}}{2}$ and $\frac{15-\sqrt{221}}{2}$, respectively. And the corresponding eigenvectors of these eigenvalues are $T_1 = \begin{pmatrix} 11+\sqrt{221} \\ 10 \end{pmatrix}$ and $T_2 = \begin{pmatrix} 11-\sqrt{221} \\ 10 \end{pmatrix}$.

Let $T = \begin{pmatrix} 11+\sqrt{221} & 11-\sqrt{221} \\ 10 & 10 \end{pmatrix}$. Then the inverse matrix of T is $T^{-1} = \begin{pmatrix} \frac{\sqrt{221}}{442} & \frac{221-11\sqrt{221}}{4420} \\ -\frac{\sqrt{221}}{442} & \frac{221+11\sqrt{221}}{4420} \end{pmatrix}$. By the property of a similarity matrix, we have

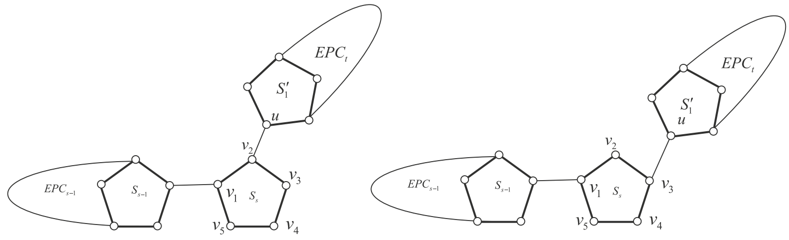

Figure 5. Two edge-pentagon-chains $EPC_s \overset{o}{\bigotimes} EPC_t$ and $EPC_s \overset{m}{\bigotimes} EPC_t$.

$$T^{-1}MT = \begin{pmatrix} \frac{15+\sqrt{221}}{2} & 0 \\ 0 & \frac{15-\sqrt{221}}{2} \end{pmatrix}.$$

So,

$$M = T \begin{pmatrix} \frac{15+\sqrt{221}}{2} & 0 \\ 0 & \frac{15+\sqrt{221}}{2} \end{pmatrix} T^{-1}. \tag{4}$$

By (3) and (4), we have

$$PS(EPC_n^m) = \frac{640237 + 43067\sqrt{221}}{442}\left(\frac{15+\sqrt{221}}{2}\right)^{n-3} + \frac{640237 - 43067\sqrt{221}}{442}\left(\frac{15-\sqrt{221}}{2}\right)^{n-3}.$$

□

Definition 2.1 Let $EPC_s = S_1S_2 \ldots S_s (s > 1)$ and $EPC_t = S'_1S'_2 \ldots S'_t$ be two edge-pentagon-chains. Suppose that $S_s = v_1v_2v_3v_4v_5$ in EPC_s and u is a vertex of S'_1 in EPC_t. $EPC_s \overset{o}{\bigotimes} EPC_t$ is an edge-pentagon-chain obtained by attaching vertex u of S'_1 in EPC_t to a ortho-vertex of S_s in EPC_s. $EPC_s \overset{m}{\bigotimes} EPC_t$ is also an edge-pentagon-chain obtained by attaching vertex u of S'_1 in EPC_t to a meta-vertex of S_s in EPC_s. The resulting graphs see Fig. 5. We designate the transformation from $EPC_s \overset{m}{\bigotimes} EPC_t$ to $EPC_s \overset{o}{\bigotimes} EPC_t$ as type **I**.

Theorem 2.1 *Let $EPC_s \overset{m}{\bigotimes} EPC_t$ and $EPC_s \overset{o}{\bigotimes} EPC_t$ be two edge-pentagon-chains defined in Definition 2.1. Then*

$$PS(EPC_s \overset{o}{\bigotimes} EPC_t) > PS(EPC_s \overset{m}{\bigotimes} EPC_t).$$

Proof Let $w \in V(EPC_{s-1})$ be the neighbor of v_1 in EPC_s. By Lemma 1.2, we obtain that

$$\begin{aligned} &PS(EPC_s \overset{o}{\bigotimes} EPC_t) \\ &= PS(EPC_{s-1})[PS(C_5)PS(EPC_t) + PS(P_4)PS(EPC_t - u)] \\ &\quad + PS(EPC_{s-1} - w)[PS(P_4)PS(EPC_t) + PS(P_3)PS(EPC_t - u)] \\ &= 13PS(EPC_{s-1})PS(EPC_t) + 5PS(EPC_{s-1})PS(EPC_t - u) \\ &\quad + 5PS(EPC_{s-1} - w)PS(EPC_t) + 3PS(EPC_{s-1} - w)PS(EPC_t - u) \end{aligned}$$

and

$$\begin{aligned} &PS(EPC_s \overset{m}{\bigotimes} EPC_t) \\ &= PS(EPC_{s-1})[PS(C_5)PS(EPC_t) + PS(P_4)PS(EPC_t - u)] \\ &\quad + PS(EPC_{s-1} - w)[PS(P_4)PS(EPC_t) + PS(P_1)PS(P_2)PS(EPC_t - u)] \\ &= 13PS(EPC_{s-1})PS(EPC_t) + 5PS(EPC_{s-1})PS(EPC_t - u) \\ &\quad + 5PS(EPC_{s-1} - w)PS(EPC_t) + 2PS(EPC_{s-1} - w)PS(EPC_t - u). \end{aligned}$$

Thus $PS(EPC_s \overset{o}{\bigotimes} EPC_t) - PS(EPC_s \overset{m}{\bigotimes} EPC_t) = PS(EPC_{s-1} - w)PS(EPC_t - u) > 0$. □

Let $\mathscr{G}_n$ be a collection of all edge-pentagon-chains EPC_n with n pentagons.

Theorem 2.2 *Let $G \in \mathscr{G}_n$ be an edge-pentagon-chain with $n \geq 3$ pentagons. Then*

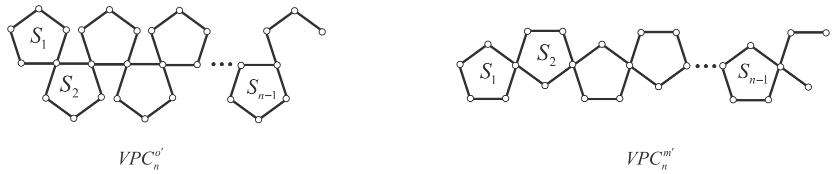

Figure 6. A vertex-ortho-pentagon-chain $VPC_n^{o'}$ and a vertex-meta-pentagon-chain $VPC_n^{m'}$.

$$\frac{640237+43067\sqrt{221}}{442}\left(\frac{15+\sqrt{221}}{2}\right)^{n-3}+\frac{640237-43067\sqrt{221}}{442}\left(\frac{15-\sqrt{221}}{2}\right)^{n-3}\le PS(G)$$
$$\le\frac{194+137\sqrt{2}}{2}\left(8+5\sqrt{2}\right)^{n-2}+\frac{194-137\sqrt{2}}{2}\left(8-5\sqrt{2}\right)^{n-2},$$

where the first equality holds if and only if $G\cong EPC_n^m$, and the second equality holds if and only if $G\cong EPC_n^o$.

Proof Let $G=S_1S_2\dots S_n\in\mathscr{G}_n$ be the edge-pentagon-chain with the smallest permanental sum. We show that $G=EPC_n^m$. Suppose to the contrary that $G\neq EPC_n^m$. Then there must exist $i\in(1,2,\dots,n)$ such that $G=EPC_i\overset{o}{\bigotimes}EPC_{n-i}$. By Theorem 2.1, there exists $G'=EPC_i\overset{m}{\bigotimes}EPC_{n-i}$ such that $PS(G')<PS(G)$, which contradicts the hypothesis G attains the minimum permanental sum. Thus, $G=EPC_n^m$.

Similarly, let $G=S_1S_2\dots S_n\in\mathscr{G}_n$ be the edge-pentagon-chain with the largest permanental sum. The following we prove that $G=EPC_n^o$. Suppose to the contrary that $G\neq EPC_n^o$. Then there must exist $i\in(1,2,\dots,n)$ such that $G=EPC_i\overset{m}{\bigotimes}EPC_{n-i}$. By Theorem 2.1, there exists $G'=EPC_i\overset{o}{\bigotimes}EPC_{n-i}$ such that $PS(G')>PS(G)$, which contradicts the hypothesis G attains the maximum permanental sum. Thus, $G=EPC_n^o$.

By Lemma 2.1 and argument as above, direct yields Theorem 2.2. □

The bound of permanental sum of vertex-pentagon-chains. We first present two auxiliary graphs. One is denoted by $VPC_n^{o'}$ obtained from VPC_n^o deleting a ortho-vertex in S_n. The other is denoted by $VPC_n^{m'}$ obtained from VPC_n^m deleting meta-vertex in S_n. The resulting graphs see Fig. 6.

Lemma 2.2 *Let VPC_n^o and VPC_n^m be a vertex-meta-pentagon-chain and a vertex-orth-pentagon-chain, respectively. Then*

$$PS(VPC_n^o)=\frac{1575+157\sqrt{105}}{30}\left(\frac{7+\sqrt{105}}{2}\right)^{n-2}+\frac{1575-157\sqrt{105}}{30}\left(\frac{7-\sqrt{105}}{2}\right)^{n-2},$$
$$PS(VPC_n^m)=\frac{14501+3517\sqrt{17}}{34}\left(4+\sqrt{17}\right)^{n-3}+\frac{14501-3517\sqrt{17}}{34}\left(4-\sqrt{17}\right)^{n-3}.$$

Proof By Lemma 1.2, we have

$$PS(VPC_n^o)=5PS(VPC_{n-1}^o)+8PS(VPC_{n-1}^{o'}),$$
$$PS(VPC_n^{o'})=3PS(VPC_{n-1}^o)+2PS(VPC_{n-1}^{o'}).$$

Thus,

$$\begin{pmatrix}PS(VPC_n^o)\\PS(VPC_n^{o'})\end{pmatrix}=\begin{pmatrix}5&8\\3&2\end{pmatrix}\begin{pmatrix}PS(VPC_{n-1}^o)\\PS(VPC_{n-1}^{o'})\end{pmatrix}.$$

Direct computation yields $PS(VPC_2^o)=105$ and $PS(VPC_2^o)=49$. Now,

$$\begin{aligned}PS(VPC_n^o)&=5PS(VPC_{n-1}^o)+8PS(VPC_{n-1}^{o'}),\\&=(5\ 8)\begin{pmatrix}5&8\\3&2\end{pmatrix}\begin{pmatrix}PS(VPC_{n-2}^o)\\PS(VPC_{n-2}^{o'})\end{pmatrix}\\&=\cdots\\&=(5\ 8)\begin{pmatrix}5&8\\3&2\end{pmatrix}^{n-3}\begin{pmatrix}105\\49\end{pmatrix}.\end{aligned}\tag{5}$$

Set matrix $M=\begin{pmatrix}5&8\\3&2\end{pmatrix}$. Then the eigenvalues of M are $\frac{7+\sqrt{105}}{2}$ and $\frac{7-\sqrt{105}}{2}$, respectively. And the corresponding eigenvectors of these eigenvalues are $T_1=\begin{pmatrix}16\\\sqrt{105}-3\end{pmatrix}$ and $T_2=\begin{pmatrix}-16\\\sqrt{105}+3\end{pmatrix}$.

Let $T=\begin{pmatrix} 16 & -16 \\ \sqrt{105}-3 & \sqrt{105}+3 \end{pmatrix}$. Then the inverse matrix of T is $T^{-1}=\begin{pmatrix} \frac{\sqrt{105}+35}{1120} & \frac{\sqrt{105}}{210} \\ \frac{\sqrt{105}-35}{1120} & \frac{\sqrt{105}}{210} \end{pmatrix}$. According to the property of a similarity matrix, we have

$$T^{-1}MT=\begin{pmatrix} \frac{7+\sqrt{105}}{2} & 0 \\ 0 & \frac{7-\sqrt{105}}{2} \end{pmatrix}.$$

So,

$$M=T\begin{pmatrix} \frac{7+\sqrt{105}}{2} & 0 \\ 0 & \frac{7-\sqrt{105}}{2} \end{pmatrix}T^{-1}. \tag{6}$$

By (5) and (6), we have

$$PS(VPC_n^o)=\frac{1575+157\sqrt{105}}{30}\left(\frac{7+\sqrt{105}}{2}\right)^{n-2}+\frac{1575-157\sqrt{105}}{30}\left(\frac{7-\sqrt{105}}{2}\right)^{n-2}.$$

Similarly, by Lemma 1.2, we obtain

$$PS(VPC_n^m)=5PS(VPC_{n-1}^m)+8PS(VPC_{n-1}^{m'}),$$
$$PS(VPC_n^{m'})=2PS(VPC_{n-1}^m)+3PS(VPC_{n-1}^{m'}).$$

So,

$$\begin{pmatrix} PS(VPC_n^m) \\ PS(VPC_n^{m'}) \end{pmatrix}=\begin{pmatrix} 5 & 8 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} PS(VPC_{n-1}^m) \\ PS(VPC_{n-1}^{m'}) \end{pmatrix}.$$

Direct computation yields $PS(VPC_2^m)=105$ and $PS(VPC_2^m)=41$. Then

$$\begin{aligned} PS(VPC_n^m)&=5PS(VPC_{n-1}^m)+8PS(VPC_{n-1}^{m'}) \\ &=(5\ 8)\begin{pmatrix} 5 & 8 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} PS(VPC_{n-2}^m) \\ PS(VPC_{n-2}^{m'}) \end{pmatrix} \\ &=\cdots \\ &=(5\ 8)\begin{pmatrix} 5 & 8 \\ 2 & 3 \end{pmatrix}^{n-3}\begin{pmatrix} 105 \\ 41 \end{pmatrix}. \end{aligned} \tag{7}$$

Let $M=\begin{pmatrix} 5 & 8 \\ 2 & 3 \end{pmatrix}$ be a matrix. Then the eigenvalues of M are $4+\sqrt{17}$ and $4-\sqrt{17}$, respectively. And the corresponding eigenvectors of these eigenvalues are $T_1=\begin{pmatrix} 1+\sqrt{17} \\ 2 \end{pmatrix}$ and $T_2=\begin{pmatrix} 1-\sqrt{17} \\ 2 \end{pmatrix}$.

Let $T=\begin{pmatrix} 1+\sqrt{17} & 1-\sqrt{17} \\ 2 & 2 \end{pmatrix}$. Then the inverse matrix of T is $T^{-1}=\begin{pmatrix} \frac{\sqrt{17}}{34} & \frac{17-\sqrt{17}}{68} \\ -\frac{\sqrt{17}}{34} & \frac{17+\sqrt{17}}{68} \end{pmatrix}$. By the property of a similarity matrix, we have

$$T^{-1}MT=\begin{pmatrix} 4+\sqrt{17} & 0 \\ 0 & 4-\sqrt{17} \end{pmatrix}.$$

Therefore,

$$M=T\begin{pmatrix} 4+\sqrt{17} & 0 \\ 0 & 4-\sqrt{17} \end{pmatrix}T^{-1}. \tag{8}$$

By (7) and (8), we have

$$PS(VPC_n^m)=\frac{14501+3517\sqrt{17}}{34}\left(4+\sqrt{17}\right)^{n-3}+\frac{14501-3517\sqrt{17}}{34}\left(4-\sqrt{17}\right)^{n-3}.$$

□

Definition 2.2 *Let $VPC_s=S_1S_2\ldots S_s(s>1)$ and $VPC_t=S_1'S_2'\ldots S_t'$ be two vertex-pentagon-chains. Suppose that $S_s=v_1v_2v_3v_4v_5$ in VPC_s and u is a vertex of S_1' in VPC_t. $VPC_s\overset{o}{\bigotimes}VPC_t$ is a vertex-pentagon-chain obtained by splicing vertex u of S_1' in VPC_t to a ortho-vertex of S_s in VPC_s. $VPC_s\overset{m}{\bigotimes}VPC_t$ is also a vertex-pentagon-chain obtained by splicing vertex u of S_1' in VPC_t to a meta-vertex of S_s in VPC_s. The resulting graphs see Fig. 7. We designate the transformation from $VPC_s\overset{m}{\bigotimes}VPC_t$ to $VPC_s\overset{o}{\bigotimes}VPC_t$ as type* **II**.

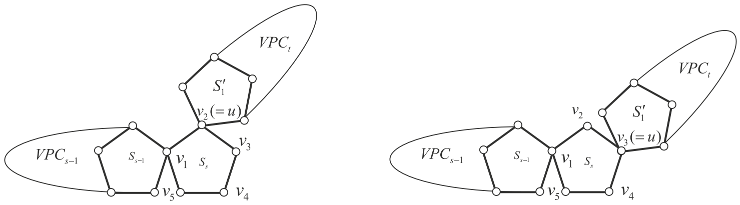

Figure 7. Two vertex-pentagon-chains $VPC_s \overset{o}{\bigotimes} VPC_t$ and $VPC_s \overset{m}{\bigotimes} VPC_t$.

Theorem 2.3 *Let $VPC_s \overset{m}{\bigotimes} VPC_t$ and $VPC_s \overset{o}{\bigotimes} VPC_t$ be two vertex-pentagon-chains defined in Definition 2.2. Then*

$$PS(VPC_s \overset{o}{\bigotimes} VPC_t) > PS(VPC_s \overset{m}{\bigotimes} VPC_t).$$

Proof Let $w_1, w_2 \in V(S'_1)$ be two neighbors of u in VPC_t. By Lemma 1.2, we obtain that

$$\begin{aligned} PS(VPC_s \overset{o}{\bigotimes} VPC_t) &= PS(VPC_s - v_2)PS(VPC_t - u) + PS(VPC_s - v_2)[PS(VPC_t \\ &\quad - u - w_1) + PS(VPC_t - u - w_2)] + [PS(VPC_s - v_2 - v_1) \\ &\quad + PS(VPC_s - v_2 - v_3)]PS(VPC_t - u) + 2PS(VPC_s - v_2) \\ &\quad PS(VPC_t - V(S'_1)) + 2PS(VPC_s - V(S_s))PS(VPC_t - u) \\ &= [5PS(VPC_{s-1}) + 6PS((VPC_{s-1} - v_1))]PS(VPC_t - u) \\ &\quad + [3PS(VPC_{s-1}) + 2PS((VPC_{s-1} - v_1))][PS(VPC_t - u - w_1) \\ &\quad + PS(VPC_t - u - w_2) + 2PS(VPC_t - V(S'_1))] \\ &\quad + 2PS(VPC_s - V(S_s))PS(VPC_t - u) \end{aligned}$$

and

$$\begin{aligned} PS(VPC_s \overset{m}{\bigotimes} VPC_t) &= PS(VPC_s - v_3)PS(VPC_t - u) + PS(VPC_s - v_3)[PS(VPC_t \\ &\quad - u - w_1) + PS(VPC_t - u - w_2)] + [PS(VPC_s - v_3 - v_2) \\ &\quad + PS(VPC_s - v_3 - v_4)]PS(VPC_t - u) + 2PS(VPC_s - v_3) \\ &\quad PS(VPC_t - V(S'_1)) + 2PS(VPC_s - V(S_s))PS(VPC_t - u) \\ &= [5PS(VPC_{s-1}) + 6PS((VPC_{s-1} - v_1))]PS(VPC_t - u) \\ &\quad + [2PS(VPC_{s-1}) + 3PS((VPC_{s-1} - v_1))][PS(VPC_t - u - w_1) \\ &\quad + PS(VPC_t - u - w_2) + 2PS(VPC_t - V(S'_1))] \\ &\quad + 2PS(VPC_s - V(S_s))PS(VPC_t - u). \end{aligned}$$

By Corollary 1.1 and argument as above, we have

$$\begin{aligned} &PS(VPC_s \overset{o}{\bigotimes} VPC_t) - PS(VPC_s \overset{m}{\bigotimes} VPC_t) \\ &= [PS(VPC_{s-1}) - PS((VPC_{s-1} - v_1))][PS(VPC_t - u - w_1) + PS(VPC_t - u - w_2) \\ &\quad + 2PS(VPC_t - V(S'_1))] > 0. \end{aligned}$$

□

Let $\mathcal{G}_n$ be a set of consisting all VPC_n with n pentagons.

Theorem 2.4 *Let $G \in \mathcal{G}_n$ be a vertex-pentagon-chain with n pentagons. Then*

$$\begin{aligned} &\frac{14501 + 3517\sqrt{17}}{34}\left(4 + \sqrt{17}\right)^{n-3} + \frac{14501 - 3517\sqrt{17}}{34}\left(4 - \sqrt{17}\right)^{n-3} \le PS(G) \\ &\le \frac{1575 + 157\sqrt{105}}{30}\left(\frac{\sqrt{105} + 7}{2}\right)^{n-2} + \frac{1575 - 157\sqrt{105}}{30}\left(\frac{\sqrt{105} - 7}{2}\right)^{n-2}, \end{aligned}$$

where the left equality holds if and only if $G \cong VPC_n^m$, and the right equality holds if and only if $G \cong VPC_n^o$.

Proof Let $G = S_1S_2 \dots S_n \in \mathcal{G}_n$ be the vertex-pentagon-chain with the smallest permanental sum. We show that $G = VPC_n^m$. Suppose to the contrary that $G \neq VPC_n^m$. Then there must exist $i \in (1, 2, \dots, n)$ such that

$G = VPC_i \overset{o}{\otimes} VPC_{n-i}$. By Theorem 2.3, there exists $G' = VPC_i \overset{m}{\otimes} VPC_{n-i}$ such that $PS(G') < PS(G)$, which contradicts the hypothesis G attains the minimum permanental sum. Thus, $G = VPC_n^m$.

Similarly, let $G = S_1S_2 \ldots S_n \in \mathscr{G}_n$ be the vertex-pentagon-chain with the largest permanental sum. The following we prove that $G = VPC_n^o$. Suppose to the contrary that $G \neq VPC_n^o$. Then there must exist $i \in (1, 2, \ldots, n)$ such that $G = VPC_i \overset{m}{\otimes} VPC_{n-i}$. By Theorem 2.1, there exists $G' = VPC_i \overset{o}{\otimes} VPC_{n-i}$ such that $PS(G') > PS(G)$, which contradicts the hypothesis G attains the maximum permanental sum. Thus, $G = VPC_n^o$.

By Lemma 2.2 and argument as above, it is straightforward to obtain Theorem 2.4. □

Discussions

Determining extremal value is an important problem in scientific research. In this paper, we characterize the tight bound of permanental sums of all edge-pentagon-chains and vertex-pentagon-chains, respectively. And the corresponding graphs are also determined. For an edge-pentagon-chain(resp. vertex-pentagon-chain), using the computing method in Lemma 2.1(resp. Lemma 2.2) can compute the permanental sum of any edge-pentagon-chain(resp. vertex-pentagon-chain). For every organic polymers, we always find a graph model corresponding it. Thus, the permanental sum of a organic polymers can be computed by the formulas in Lemma 1.2.

$C_{50}(D_{5h})$ is captured and its permanental sum achieves the minimum among all C_{50}. Is the phenomenon a coincidence? Does the phenomenon exist for other chemical molecular? These are very interesting problems. However, we cannot answer them. Our motivation is to determine the extremal graphs with respect to permanental sum for some type chemical graphs in this paper. In the future, we will find the answers of the problem as above.

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Competing interests
The authors declare no competing interests.

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