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

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

where the sum is taken over all permutations $\sigma$ 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

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

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. Cash3 investigated permanental polynomials of some chemical graphs(including benzene, o-biphenylene, coronene, C20 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 published4-14. 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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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 $EPC_n^m$.

The resulting graphs see Fig. 2. Contracting every cut edge in $VPC_n$, the resulting graphs $VPC_{n-1}$, respectively. See Fig. 3.

Let $P_n$ be a path with $n$ vertices. Then

**Lemma 1.1**  

1. Let $P_n$ be a path with $n$ vertices.
where 
\[ F(0) = 0, \quad F(1) = 1 \quad \text{and} \quad F(n) = F(n-1) + F(n-2) \] 
for \( n \geq 2 \) denotes the sequence of Fibonacci numbers.

**Lemma 1.2**

The permanental sum of a graph satisfies the following identities:

(i) Let \( G \) and \( H \) be two connected graphs. Then

\[
PS(G \cup H) = PS(G) \cdot PS(H).
\]

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

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

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

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

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 \( EPC_n^m \) deleting a ortho-vertex in \( S_n \). The other is denoted by \( EPC_m^m \) obtained from \( EPC_m^m \) deleting meta-vertex in \( S_n \). The resulting graphs see Fig. 4.

**Lemma 2.1**

Let \( EPC_n^o \) and \( EPC_m^m \) be an edge-ortho-pentagon-chain and an edge-meta-pentagon-chain, respectively. Then

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

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

**Proof**

By Lemma 1.2, we have

\[
PS(EPC_n^o) = 13PS(EPC_{n-1}^o) + 5PS(EPC_{n-1}^d),
\]

\[
PS(EPC_n^m) = 5PS(EPC_{n-1}^o) + 3PS(EPC_{n-1}^d).
\]

Thus,
\[
\begin{pmatrix}
PS(\text{EPC}_n^o) \\
PS(\text{EPC}_n^2)
\end{pmatrix} = \begin{pmatrix} 13 & 5 \\ 5 & 3 \end{pmatrix} \begin{pmatrix} PS(\text{EPC}_{n-1}^o) \\
PS(\text{EPC}_{n-1}^2) \end{pmatrix}.
\]

Direct computation yields \(PS(\text{EPC}_2^2) = 194\) and \(PS(\text{EPC}_3^2) = 80\). Now,
\[
PS(\text{EPC}_n^o) = 13PS(\text{EPC}_{n-1}^o) + 5PS(\text{EPC}_{n-1}^2),
\]
\[
= (13 \ 5) \begin{pmatrix} PS(\text{EPC}_{n-2}^o) \\
PS(\text{EPC}_{n-2}^2) \end{pmatrix}
\]
\[
= \ldots
\]
\[
= (13 \ 5) \begin{pmatrix} 13 & 5 \\ 5 & 3 \end{pmatrix}^{n-3} \begin{pmatrix} 194 \\
80 \end{pmatrix}.
\]

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 \(T = \begin{pmatrix} 1 \\
\sqrt{2} - 1 \ 1 \end{pmatrix}\). Then the inverse matrix of \(T\) is \(T^{-1} = \begin{pmatrix} \sqrt{2} + 2 \\
2 - \sqrt{2} \end{pmatrix}\). 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,
\[
M = T \begin{pmatrix} 8 + 5\sqrt{2} & 0 \\
0 & 8 - 5\sqrt{2} \end{pmatrix} T^{-1}.
\]

By (1) and (2), we have
\[
PS(\text{EPC}_n^o) = (13 \ 5) \begin{pmatrix} 1 \\ \sqrt{2} - 1 \ 1 \end{pmatrix} \begin{pmatrix} 8 + 5\sqrt{2} & 0 \\
0 & 8 - 5\sqrt{2} \end{pmatrix} \begin{pmatrix} \sqrt{2} + 2 \\
2 - \sqrt{2} \end{pmatrix} \begin{pmatrix} 194 \\
80 \end{pmatrix}
\]
\[
= \begin{pmatrix} 194 + 137\sqrt{2} \\
2 \end{pmatrix} (8 + 5\sqrt{2})^{n-2} + \begin{pmatrix} 194 - 137\sqrt{2} \\
2 \end{pmatrix} (8 - 5\sqrt{2})^{n-2}.
\]

Similarly, by Lemma 1.2, we obtain
\[
PS(\text{EPC}_n^m) = 13PS(\text{EPC}_{n-1}^m) + 5PS(\text{EPC}_{n-1}^m),
\]
\[
PS(\text{EPC}_n^m) = 5PS(\text{EPC}_{n-1}^m) + 2PS(\text{EPC}_{n-1}^m).
\]

So,
\[
\begin{pmatrix} PS(\text{EPC}_n^m) \\
PS(\text{EPC}_n^m) \end{pmatrix} = \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix} \begin{pmatrix} PS(\text{EPC}_{n-1}^m) \\
PS(\text{EPC}_{n-1}^m) \end{pmatrix}.
\]

Direct computation yields \(PS(\text{EPC}_2^m) = 194\) and \(PS(\text{EPC}_3^m) = 75\). Then,
\[
PS(\text{EPC}_n^m) = 13PS(\text{EPC}_{n-1}^m) + 5PS(\text{EPC}_{n-1}^m),
\]
\[
= (13 \ 5) \begin{pmatrix} PS(\text{EPC}_{n-2}^m) \\
PS(\text{EPC}_{n-2}^m) \end{pmatrix}
\]
\[
= \ldots
\]
\[
= (13 \ 5) \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix}^{n-3} \begin{pmatrix} 194 \\
75 \end{pmatrix}.
\]

Let \(M = \begin{pmatrix} 13 & 5 \\ 5 & 2 \end{pmatrix}\) be a matrix. Then the eigenvalues of \(M\) are \(15 + \sqrt{221}\) and \(15 - \sqrt{221}\), 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 \(T = \begin{pmatrix} 11 + \sqrt{221} \\
10 \end{pmatrix} \begin{pmatrix} 11 - \sqrt{221} \\
10 \end{pmatrix}\). Then the inverse matrix of \(T\) is \(T^{-1} = \begin{pmatrix} \frac{221 + 11\sqrt{221}}{440} \\
\frac{221 - 11\sqrt{221}}{440} \end{pmatrix}\). By the property of a similarity matrix, we have
Theorem 2.2 obtained by attaching vertex $u$

Let $\mathbf{S}$ be a collection of all edge-pentagon-chains $EPC_{\sigma}$ and $EPC_{\tau}$.

Figure 5. Two edge-pentagon-chains $EPC_{\sigma} \circ EPC_{\tau}$ and $EPC_{\tau} \circ EPC_{\sigma}$.

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

So,

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

By (3) and (4), we have

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

\[\square\]

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

Theorem 2.1 Let $EPC_{\sigma} \circ EPC_{\tau}$ and $EPC_{\tau} \circ EPC_{\sigma}$ be two edge-pentagon-chains defined in Definition 2.1. Then

$$PS(EPC_{\tau} \circ EPC_{\sigma}) > PS(EPC_{\sigma} \circ EPC_{\tau}).$$

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

$$PS(EPC_{\tau} \circ EPC_{\sigma})$$

$$= PS(EPC_{\sigma-1})[PS(C_0)PS(EPC_{\tau}) + PS(P_1)PS(EPC_{\tau} - u)]$$

$$+ PS(EPC_{\sigma-1} - w) [PS(P_1)PS(EPC_{\tau}) + PS(P_2)PS(EPC_{\tau} - u)]$$

$$= 13PS(EPC_{\sigma-1})PS(EPC_{\tau}) + 5PS(EPC_{\sigma-1})PS(EPC_{\tau} - u)$$

$$+ 5PS(EPC_{\sigma-1} - w)PS(EPC_{\tau}) + 3PS(EPC_{\sigma-1} - w)PS(EPC_{\tau} - u)$$

and

$$PS(EPC_{\sigma} \circ EPC_{\tau})$$

$$= PS(EPC_{\sigma-1})[PS(C_0)PS(EPC_{\tau}) + PS(P_1)PS(EPC_{\tau} - u)]$$

$$+ PS(EPC_{\sigma-1} - w) [PS(P_1)PS(EPC_{\tau}) + PS(P_2)PS(EPC_{\tau} - u)]$$

$$= 13PS(EPC_{\sigma-1})PS(EPC_{\tau}) + 5PS(EPC_{\sigma-1})PS(EPC_{\tau} - u)$$

$$+ 5PS(EPC_{\sigma-1} - w)PS(EPC_{\tau}) + 2PS(EPC_{\sigma-1} - w)PS(EPC_{\tau} - u).$$

Thus $PS(EPC_{\tau} \circ EPC_{\sigma}) - PS(EPC_{\sigma} \circ EPC_{\tau}) = PS(EPC_{\sigma-1} - w)PS(EPC_{\tau} - u) > 0.$

\[\square\]

Let $G_n$ be a collection of all edge-pentagon-chains $EPC_n$ with $n$ pentagons.

Theorem 2.2 Let $G \in G_n$ be an edge-pentagon-chain with $n \geq 3$ pentagons. Then
640237 + 43067\sqrt{221} \quad \frac{15 + \sqrt{221}}{2}^{n-3} + \frac{640237 - 43067\sqrt{221}}{2}^{n-3} \quad \leq PS(G)
\leq \frac{194 + 137\sqrt{2}}{2} \quad (8 + 5\sqrt{2})^{n-2} + \frac{194 - 137\sqrt{2}}{2} \quad (8 - 5\sqrt{2})^{n-2},
where the first equality holds if and only if G \equiv EPC^m_n, and the second equality holds if and only if G \equiv EPC^o_n.

**Proof** Let G = S_1S_2...S_n \in \mathscr{G}_n be the edge-pentagon-chain with the smallest permanental sum. We show that G = EPC^m_n. Suppose to the contrary that G \neq EPC^m_n. Then there must exist i \in (1, 2, ..., n) such that G = EPC^m_i \otimes EPC_n\setminus_i. By Theorem 2.1, there exists G' = EPC^m_i \otimes EPC_n\setminus_{i+1} such that PS(G') < PS(G), which contradicts the hypothesis G attains the minimum permanental sum. Thus, G = EPC^m_n.

Similarly, let G = S_1S_2...S_n \in \mathscr{G}_n be the edge-pentagon-chain with the largest permanental sum. The following we prove that G = EPC^o_n. Suppose to the contrary that G \neq EPC^o_n. Then there must exist i \in (1, 2, ..., n) such that G = EPC^o_i \otimes EPC_n\setminus_i. By Theorem 2.1, there exists G' = EPC^o_i \otimes EPC_n\setminus_{i+1} such that PS(G') > PS(G), which contradicts the hypothesis G attains the maximum permanental sum. Thus, G = EPC^o_n.

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

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**The bound of permanental sum of vertex-pentagon-chains.** We first present two auxiliary graphs. One is denoted by VPC^o_n obtained from VPC^m_n deleting a ortho-vertex in S_n. The other is denoted by VPC^m_n obtained from VPC^m_n deleting meta-vertex in S_n. The resulting graphs see Fig. 6.

**Lemma 2.2** Let VPC^o_n and VPC^m_n be a vertex-meta-pentagon-chain and a vertex-orth-pentagon-chain, respectively. Then
\[
PS(VPC^o_n) = \frac{1575 + 157\sqrt{105}}{30} \quad \left(7 + \sqrt{105}\right)\quad n-2 + \frac{1575 - 157\sqrt{105}}{30} \quad \left(7 - \sqrt{105}\right)\quad n-2,
PS(VPC^m_n) = \frac{14501 + 3517\sqrt{17}}{34} \quad \left(4 + \sqrt{17}\right)\quad n-3 + \frac{14501 - 3517\sqrt{17}}{34} \quad \left(4 - \sqrt{17}\right)\quad n-3.
\]

**Proof** By Lemma 1.2, we have
\[
PS(VPC^o_n) = 5PS(VPC^o_{n-1}) + 8PS(VPC^o_{n-1}),
PS(VPC^o_n) = 3PS(VPC^o_{n-1}) + 2PS(VPC^o_{n-1}).
\]

Thus,
\[
\left(\frac{PS(VPC^o_n)}{PS(VPC^o_n)}\right) = \begin{pmatrix} 5 & 8 \\ 3 & 2 \end{pmatrix} \quad \left(\frac{PS(VPC^o_{n-1})}{PS(VPC^o_{n-2})}\right).
\]

Direct computation yields PS(VPC^o_2) = 105 and PS(VPC^o_3) = 49. Now,
\[
PS(VPC^o_n) = 5PS(VPC^o_{n-1}) + 8PS(VPC^o_{n-2}),
= 5 \cdot 8 \quad \begin{pmatrix} 5 & 8 \\ 3 & 2 \end{pmatrix} \quad \left(\frac{PS(VPC^o_{n-2})}{PS(VPC^o_{n-3})}\right)
= \cdots
= 5 \cdot 8 \quad \begin{pmatrix} 5 & 8 \\ 3 & 2 \end{pmatrix} \quad n-3 \quad \begin{pmatrix} 105 \\ 49 \end{pmatrix}.
\]

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 \( T_1 = \left( \frac{16}{\sqrt{105} - 3} \right) \) and \( T_2 = \left( \frac{-16}{\sqrt{105} + 3} \right) \).
Let $T = \left(\begin{array}{cc} 16 & -16 \\ \sqrt{105} - 3 & \sqrt{105} + 3 \end{array}\right)$. Then the inverse matrix of $T$ is $T^{-1} = \left(\begin{array}{cc} \sqrt{105} + 36 & -\sqrt{105} \\ 1120 & \sqrt{105} + 32 \end{array}\right)$. According to the property of a similarity matrix, we have

$$T^{-1}MT = \left(\begin{array}{cc} \frac{7 + \sqrt{105}}{2} & 0 \\ 0 & \frac{7 - \sqrt{105}}{2} \end{array}\right).$$

So,

$$M = T \left(\begin{array}{cc} \frac{7 + \sqrt{105}}{2} & 0 \\ 0 & \frac{7 - \sqrt{105}}{2} \end{array}\right) T^{-1}.$$

By (5) and (6), we have

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

Similarly, by Lemma 1.2, we obtain

$$PS(VPC_s^m) = 5PS(VPC_{s-1}^m) + 8PS(VPC_{s-2}^m),$$

$$PS(VPC_{s-1}^m) = 2PS(VPC_{s-1}^m) + 3PS(VPC_{s-1}^m).$$

Direct computation yields $PS(VPC_2^m) = 105$ and $PS(VPC_3^m) = 41$. Then

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

$$= (5, 8) \left(\begin{array}{cc} 5 & 8 \\ 2 & 3 \end{array}\right) \left(\begin{array}{cc} PS(VPC_{n-2}^m) \\ PS(VPC_{n-3}^m) \end{array}\right),$$

$$= \ldots$$

$$= (5, 8) \left(\begin{array}{cc} 5 & 8 \\ 2 & 3 \end{array}\right)^{n-3} \left(\begin{array}{c} 105 \\ 41 \end{array}\right).$$

Let $M = \left(\begin{array}{cc} 5 & 8 \\ 2 & 3 \end{array}\right)$ 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 $T_1 = \left(\begin{array}{c} 1 + \sqrt{17} \\ 2 \end{array}\right)$ and $T_2 = \left(\begin{array}{c} 1 - \sqrt{17} \\ 2 \end{array}\right)$.

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

$$T^{-1}MT = \left(\begin{array}{cc} 4 + \sqrt{17} & 0 \\ 0 & 4 - \sqrt{17} \end{array}\right).$$

Therefore,

$$M = T \left(\begin{array}{cc} 4 + \sqrt{17} & 0 \\ 0 & 4 - \sqrt{17} \end{array}\right) T^{-1}.$$
Theorem 2.3 Let $VPC_t \otimes VPC_t$ and $VPC_t \otimes VPC_t$ be two vertex-pentagon-chains defined in Definition 2.2. Then

$$\text{PS}(VPC_t \otimes VPC_t) > \text{PS}(VPC_t \otimes VPC_t).$$

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

$$\text{PS}(VPC_t \otimes VPC_t) = \text{PS}(VPC_t - v_1)\text{PS}(VPC_t - u) + \text{PS}(VPC_t - v_2)\text{PS}(VPC_t - u - v_1)$$

and

$$\text{PS}(VPC_t \otimes VPC_t) = \text{PS}(VPC_t - v_1)\text{PS}(VPC_t - u) + \text{PS}(VPC_t - v_2)\text{PS}(VPC_t - v_1 + \text{PS}(VPC_t - v_3)\text{PS}(VPC_t - u)$$

By Corollary 1.1 and argument as above, we have

$$\text{PS}(VPC_t \otimes VPC_t) - \text{PS}(VPC_t \otimes VPC_t)$$

Let $G_n$ be a set of consisting all $VPC_n$ with $n$ pentagons.

Theorem 2.4 Let $G \in G_n$ be a vertex-pentagon-chain with $n$ pentagons. Then

$$\frac{14501 + 35\sqrt{17}}{34} \left(4 + \sqrt{17}\right)^{n-3} + \frac{14501 - 35\sqrt{17}}{34} \left(4 - \sqrt{17}\right)^{n-3} \leq \text{PS}(G)$$

$$\leq \frac{1575 + 15\sqrt{105}}{2} \left(\frac{105 + 7}{2}\right)^{n-2} + \frac{1575 - 15\sqrt{105}}{2} \left(\frac{105 - 7}{2}\right)^{n-2},$$

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

Proof Let $G = S_1S_2 \ldots S_n \in G_n$ be the vertex-pentagon-chain with the smallest permanental sum. We show 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 (VPC_i o VPC_{m-i}). By Theorem 2.3, there exists G' = VPC_i (VPC_i o VPC_{m-i}) such that PS(G') < PS(G), which contradicts the hypothesis G attains the minimum permanent sum. Thus, G = VPC_m.

Similarly, let G = S_i S_2 ... S_n ∈ ℓ G be the vertex-pentagon-chain with the largest permanent sum. The following we prove that G = VPC_n. Suppose to the contrary that G ≠ VPC_n. Then there must exist i ∈ (1, 2, ..., n) such that G = VPC_i (VPC_i o VPC_{m-i}). By Theorem 2.1, there exists G' = VPC_i (VPC_i o VPC_{m-i}) such that PS(G') > PS(G), which contradicts the hypothesis G attains the maximum permanent sum. Thus, G = VPC_m.

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 permanent 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 permanent sum of any edge-pentagon-chain(resp. vertex-pentagon-chain). For every organic polymers, we always find a graph model corresponding it. Thus, the permanent sum of an organic polymers can be computed by the formulas in Lemma 1.2. C01(D_{56}) is captured and its permanent sum achieves the minimum among all C_{56}. 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 permanent 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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Wrote the paper: T.W., S.Z. Did the analysis: T.W., H.W., S.Z., and K.D. All authors have read and approved the final manuscript.

Competing interests
The authors declare no competing interests.

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