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Two Classes of Chains with Maximal and Minimal Total π-Electron Energy*

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Abstract. The six-membered ring spiro chain can be considered as the graph representations of an important subclass of linear unbranched, saturated spiro molecules. We prove that Z_n and S_n have the maximal and minimal energies in the set of all six-membered ring spiro chains. For the polyphenyl chains, we prove that Z_N and S_N have the maximal and minimal energies.

1. Introduction

The HMO total π-electron energy is a well-known topological index in theoretical chemistry. In fact, the experimental heats of formation of conjugated hydrocarbons are closely related to the total π-electron energy. Furthermore, it can be used to calculate the resonance energies and the results are as good as those obtained by more advanced SCF-MO methods [7].

The energy of a graph is equal to the sum of the absolute values of its eigenvalues. This concept was proposed quite some time ago in the paper: I. Gutman, The energy of a graph, *Berichte der Mathematisch-Statistischen Sektion im Forschungszentrum Graz* 103 (1978) 1-22 (and later on several other occasions). After a long latent period, it now became a popular topic of research.

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As pointed out in [7, 4], the total π-electron energy of a conjugated molecule is a bridge between the chemical structure and its thermodynamic stability. For this topic, some bounds of the total π-electron energy have been found [4, 5]. Gutman determined the trees with the maximal and minimal energy [3] and gave some further results. Since then the problem of extremal energy was solved for a variety of classes of graphs; for recent results along these lines see the recent papers [2, 6, 8–13, 15–17] and the references cited therein. Spiro compounds are an important subclass of cycloalkanes in organic chemistry. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc. (see Figure 1). Two or more benzene rings, linked by a single bond, form the polycyclic aromatic hydrocarbons (see Figure 2). A kind of compound in which two or more benzene rings are directly linked by single bonds are known as the biphenyl compounds, which play a very important role in theoretical chemistry, too.

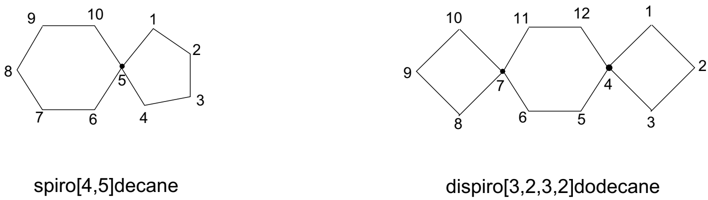

Figure 1:

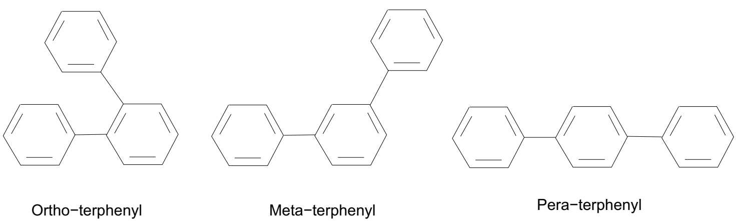

Figure 2:

In this letter, we are trying to find the extremal energies of the six-membered ring spiro chains and the polyphenyl chains. This will help the study chemical structure of spiro compounds and biphenyl compounds.

The characteristic polynomial of a graph G is denoted by Φ_G, It is well known that if

G is a bipartite graph, then Φ_G can be written as

$$\Phi_G = \sum_{k=0}^{\lfloor n/2 \rfloor} a_{2k}(G)x^{n-2k} = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b_{2k}(G)x^{n-2k} \tag{1}$$

where n is number of vertices of G. Note that $b_0(G) = 1$, $b_{2k}(G) \geq 0$ for all $k = 1, 2, \ldots, \lfloor n/2 \rfloor$. The total π-electron energy of the molecule is defined to be

$$E(G) = \sum_{j=1}^{n} |\lambda_j|$$

where λ_j , $j = 1, 2, \ldots, n$, are the eigenvalues of G. The energy of a bipartite graph G is also expressed by the Coulson integral formula [7, 4, 5, 3] as

$$E(G) = \frac{2}{\pi} \int_0^{\infty} x^{-2} \ln \left[1 + \sum_{k=0}^{\lfloor n/2 \rfloor} b_{2k}(G)x^{2k} \right] dx \ .$$

One can see that $E(G)$ is a strictly monotonously increasing function of the coefficients of the characteristic polynomial of G. This fact inspired Gutman to define a quasiordering to compare the energies of trees and further for a set of graphs.

If for two bipartite graphs G_1 and G_2 whose characteristic polynomials are of the form (1), $b_{2k}(G_1) \geq b_{2k}(G_2)$ hold for all $k \geq 0$, we say that G_1 is not less than G_2, written as $G_1 \succeq G_2$ or $G_2 \preceq G_1$. Obviously, if $G_1 \succeq G_2$ and $G_2 \preceq G_1$, then G_1 and G_2 have the same non-zero eigenvalues. If $G_1 \succeq G_2$ and there is a k such that $b_{2k}(G_1) > b_{2k}(G_2)$, then we write that $G_1 \succ G_2$. By the strict monotonicity of $E(G)$, if $G_1 \succeq G_2$ for two bipartite graphs G_1 and G_2, then $E(G_1) \geq E(G_2)$ and $E(G_1) > E(G_2)$, if $G_1 \succ G_2$, Stimulated by Refs. [14, 18], our attention turns to six-membered ring spiro chains and polyphenyl chains.

2. Six-membered ring spiro chains

2.1. Definition. *Spiro union* is a linkage between two rings that consists of a single atom common to both rings. The common atom is designated as the *spiro atom. Six-membered ring spiro chain* is a graph consisting of n six-membered ring $H_1, H_2, \ldots, H_n$, $(n \geq 1)$ with the properties that (i) for any $1 \leq k < j \leq n-1$, H_k and H_j are linked by spiro union if and only if $j = k+1$; (ii) every spiro atom belongs to at most two six-membered rings.

Obviously, "six-membered ring spiro chain" can be considered as the graph representation of an important subclass of linear unbranched, saturated multispiro molecules, in which every ring is a six-membered ring.

We denote by $\mathscr{G}_n$ the set of the six-membered ring spiro chain with n six-membered rings. Any element $G_n \in \mathscr{G}_n$ $(n \geq 1)$ can be obtained by spiro union a six-membered

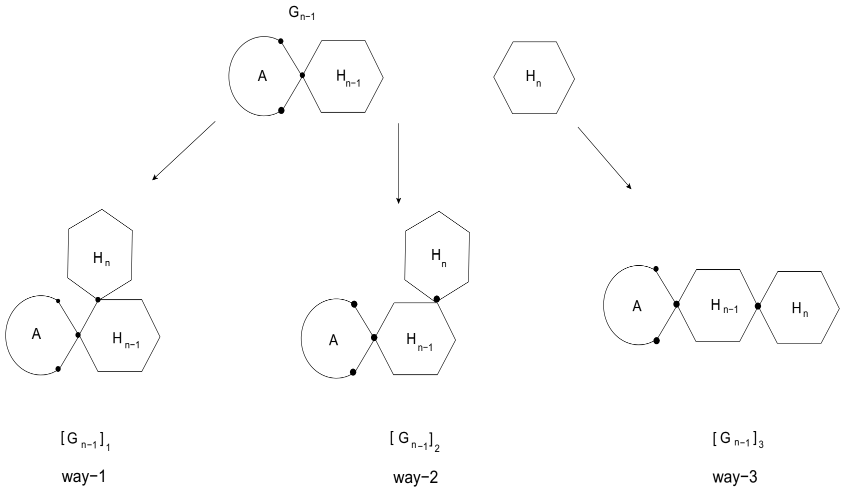

Figure 3: G_n

ring to the last six-membered ring H_{n-1} of G_{n-1}, where $G_{n-1} \in \mathscr{G}_{n-1}$. There are three non-isomorphic adding ways $G_{n-1} \to [G_{n-1}]_k = G_n$, where k=1, 2, 3; $A \in \mathscr{G}_{n-2}$ (see Figure 3). We call these three spiro union ways respectively: way-1, way-2, way-3.

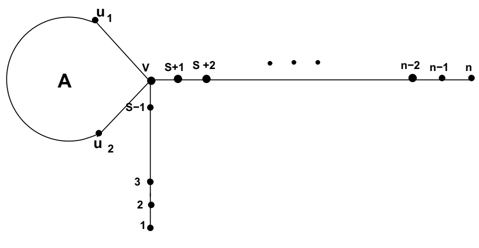

Figure 4: $H(A, s)$

In particular, if every six-membered ring in the six-membered ring spiro chain is added by the way-1, then denote by Z_n; if every six-membered ring in the six-membered ring spiro chain is added by the way-2, then denote by S_n; if every six-membered ring in the six-membered ring spiro chain is added by the way-3, then denote by L_n. In this paper, we will prove that Z_n and S_n have the maximal and minimal energies in the set of six-membered ring spiro chains.

$H(A,s)$ is the graph obtained by coinciding the s-th vertex of P_n and the atom of the last six-membered ring in the six-membered ring spiro chain $A \in \mathbf{G}_{i-1}$, $i \geq 1$ and $s = 1,2,3,\ldots,n$ (see Figure 4).

Let $A \in \mathbf{G}_{i-1}$, $B \in \mathbf{G}_{n-i}$ and H_i be the six-membered rings. G_i is obtained by spiro union of H_i to A. If B is spiro union to $G_i \in \mathbf{G}_i$ by way-k, we denote by $G_n(i,k)$, $1 \leq i \leq n-1$ and $k = 1,2,3$ (see Figure 5).

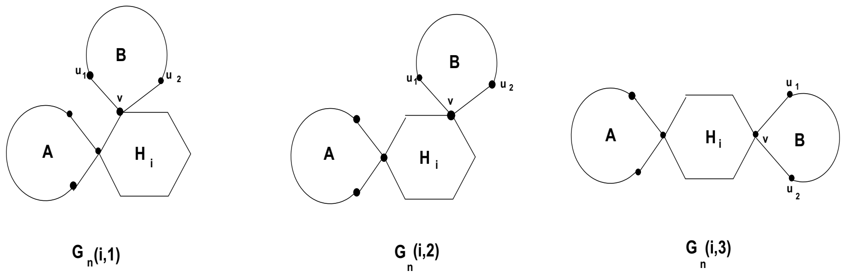

Figure 5: $G_n(i,k)$

In order to obtain the result we need some auxiliary lemmas.

2.2. Auxiliary lemmas

Lemma 2.2.1. [1]. Let uv be an edge of G. Then

$$\phi(G,\lambda) = \phi(G-uv,\lambda) - \phi(G-u-v,\lambda) - 2\sum_{C\in\xi(uv)} \phi(G-C,\lambda)$$

where $\xi(uv)$ is the set of cycles containing uv. In particular, if uv is not in any a cycle, then $\phi(G,\lambda) = \phi(G-uv,\lambda) - \phi(G-u-v,\lambda)$.

Lemma 2.2.2. [19]. Let uv be an edge of a bipartite graph G. Then

$$\begin{aligned} b_{2k}(G) &= b_{2k}(G-u-v) + b_{2k-2}(G-u-v) \\ &+ 2\sum_{C_\ell\in\xi(uv)} (-1)^{1+\ell/2}\, b_{2k-\ell}(G-C_\ell) \end{aligned}$$

where $\xi(uv)$ is the set of cycles containing uv. In particular, if uv is not in any a cycle, then

$$b_{2k}(G) = b_{2k}(G-uv) + b_{2k-2}(G-u-v)\ .$$

Proof. By Lemma 2.2.1, we have

$$a_{2k}(G) = a_{2k}(G - uv) - a_{2k-2}(G - u - v) - 2 \sum_{C_l \in \xi(uv)} a_{2k-l}(G - C_l)$$

and

$$\begin{aligned} (-1)^k a_{2k}(G) &= (-1)^k a_{2k}(G - uv) + (-1)^{k-1} a_{2k-2}(G - u - v) \\ &+ 2 \sum_{C_\ell \in \xi(uv)} (-1)^{1+\ell/2} (-1)^{k-\ell/2} a_{2k-\ell}(G - C_\ell) . \end{aligned}$$

Since $b_{2k}(G) = (-1)^k a_{2k}(G)$, the result follows. ■

The following Lemma 2.2.3 is obvious.

Lemma 2.2.3. Let G and G' be two bipartite graphs of order n with characteristic polynomials

$$\Phi(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b_{2k} x^{n-2k}$$

and

$$\Phi(G') = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b'_{2k} x^{n-2k}$$

respectively, then $G \succeq G'$ iff $b_0 = b'_0$ and $b_{2k} \geq b'_{2k}$ for $k = 1, 2, 3, \ldots, \lfloor n/2 \rfloor$. Further, $G \succ G'$ iff $G \succeq G'$ and there is a $k \in \{1, 2, \ldots, \lfloor n/2 \rfloor\}$, such that $b_{2k} > b'_{2k}$. ■

Lemma 2.2.4. [7] Let $n = 4k$, $4k+1$, $4k+2$, $4k+3$. Then $P_n \succ P_2 \bigcup P_{n-2} \succ P_4 \bigcup P_{n-4} \succ P_6 \bigcup P_{n-6} \succ \cdots \succ P_{2k} \bigcup P_{n-2k} \succ P_{2k+1} \bigcup P_{n-2k-1} \succ P_{2k-1} \bigcup P_{n-2k+1} \succ \cdots \succ P_3 \bigcup P_{n-3} \succ P_1 \bigcup P_{n-1}$.

Lemma 2.2.5. Let G_1 and G_2 be two graphs with n vertices, if $G_1 \succeq G_2$, then G$\cup G_1 \succeq G \cup G_2$; if $G_1 \succ G_2$, then G$\cup G_1 \succ G \cup G_2$.

2.3. Main result

Theorem 2.3.1. Let A $\in \mathscr{G}_{i-1}$ $(i \geq 1)$ be a six-membered ring spiro chain and P_n be a path, where $n = 4k, 4k+1, 4k+2, 4k+3$. Then $H(A,1) \succ H(A,3) \succ H(A,5) \succ \cdots \succ H(A, 2k+1) \succ H(A, 2k) \succ H(A, 2k-2) \succ \cdots \succ H(A,4) \succ H(A,2)$.

Proof. Let $u_1 v$ and $u_2 v$ be the edge in A, where v is a common vertex of A and P_n (see Figure 3). Compare the energies of two graphs, only to compare the corresponding coefficients of their characteristic polynomial by Lemma 2.2.3. By Lemma 2.2.2, we have

$$b_{2i}(H(A,s)) = b_{2i}(H(A,s) - u_1 v) + b_{2i-2}(H(A,s) - u_1 - v) + 2 b_{2i-6}(H(A,s) - H_{i-1}) .$$

It is obvious that

$$H(A,s) - u_1 - v = (A - u_1 - v)\bigcup P_{s-1}\bigcup P_{n-s}$$

and

$$H(A,s) - H_{i-1} = (A - H_{i-1})\bigcup P_{s-1}\bigcup P_{n-s}$$

so for all $s = 1, 2, \ldots, n$, we only have to consider $P_{s-1}\bigcup P_{n-s}$. By Lemma 2.2.4, we have $P_{n-1} \succ P_2\bigcup P_{n-3} \succ P_4\bigcup P_{n-5} \succ P_6\bigcup P_{n-7} \succ \cdots \succ P_{2k}\bigcup P_{n-1-2k} \succ P_{2k+1}\bigcup P_{n-2k-2} \succ P_{2k-1}\bigcup P_{n-2k} \succ \cdots \succ P_3\bigcup P_{n-4} \succ P_1\bigcup P_{n-2}$. At last, we consider $H(A,s) - u_1v$. By Lemma 2.2.2, we have

$$\begin{aligned} b_{2i}(H(A,s) - u_1v) &= b_{2i}(H(A,s) - u_1v - u_2v) + b_{2i-2}(H(A,s) - u_1v - u_2 - v) \\ &+ 2b_{2i-6}(H(A,s) - H_{i-1}) \, . \end{aligned}$$

Clearly, $H(A,s) - u_1v - u_2v = (A - u_1v - u_2v)\bigcup P_n$. So it suffices to consider $b_{2i-2}(H(A,s) - u_1v - u_2 - v)$. Obviously, $H(A,s) - u_1v - u_2 - v = (A - u_2 - v)\bigcup P_{s-1}\bigcup P_{n-s}$, and in a similar manner as in the above proof we can compare $P_{s-1}\bigcup P_{n-s}$, for all s. This completes the proof. ■

Theorem 2.3.2. $G_n(i,1) \succ G_n(i,3) \succ G_n(i,2)$.

Proof. Let u_1v and u_2v be the edge in H_{i+1}, where v is a common vertex of H_i and H_{i+1} (see Figure 4). By Lemma 2.2.2, we have

$$b_{2i}(G_n(i,k)) = b_{2i}(G_n(i,k) - u_1v) + b_{2i-2}(G_n(i,k) - u_1 - v) + 2b_{2i-6}(G_n(i,k) - H_{i+1})$$

for $k = 1, 2, 3$. Clearly, $G_n(i,k) - u_1 - v = H(A,k)\bigcup(B - u_1 - v)$. By Theorem 2.3.1 we have $H(A,1) \succ H(A,3) \succ H(A,2)$. So by Lemma 5, $G_n(i,1) - u_1 - v \succ G_n(i,3) - u_1 - v \succ G_k(i,2) - u_1 - v$. At the same time, $G_n(i,k) - H_{i+1} = H(A,k)\bigcup(B - H_{i+1})$. Similarly, we obtain that $G_n(i,1) - H_{i+1} \succ G_n(i,3) - H_{i+1} \succ G_n(i,2) - H_{i+1}$. At last, we see that

$$\begin{aligned} b_{2i}(G_n(i,k) - u_1v) &= b_{2i}(G_n(i,k) - u_1v - u_2v) + b_{2i-2}(G_n(i,k) - u_1v - u_2 - v) \\ &+ 2b_{2i-6}(G_n(i,k) - H_{i+1}) \, . \end{aligned}$$

Clearly, $G_n(i,k) - u_1v - u_2v$ are isomorphic for all $k = 1, 2, 3$, and $G_n(i,k) - u_1v - u_2 - v = H(A,k)\bigcup(B - u_1 - u_2)$ for $k = 1, 2, 3$.

Because $H(A,1) \succ H(A,3) \succ H(A,2)$ by Theorem 2.3.1, we get $G_n(i,1) - u_1v - u_2 - v \succ G_n(i,3) - u_1v - u_2 - v \succ G_k(i,2) - u_1v - u_2 - v$. The conclusion follows. ■

Theorem 2.3.3. Among all the six-membered ring spiro chains with n six-membered rings, we have $Z_n \succ L_n \succ S_n$.

Proof. We attempt to prove that Z_n and S_n are the unique maximal element and minimal element in the set of six-membered chains with n six-membered rings, respectively. We first consider the maximal energy. Let $\bar{L}_n$ be a six-membered ring spiro chain that we make the 2-th six-membered ring in L_n added to the previous six-membered ring by way-1. We get $L_n \prec \bar{L}_n$ by the Theorem 2.3.2, immediately. Repeating the approach, we can find a series of the six-membered ring spiro chains $L_n \prec \bar{L}_n \prec \bar{\bar{L}}_n \prec \cdots \prec Z_n$.

On the other hand, we find the graph with the minimal energy. Let $\tilde{L}_n$ be a six-membered ring spiro chain that we make the 2-th six-membered ring in L_n add to the previous six-membered ring by way-2. The proof of minimal energy is similar to the maximal energy. It is easy to get $L_n \succ \tilde{L}_n \succ \tilde{\tilde{L}}_n \succ \cdots \succ S_n$. Thus we proved that Z_n and S_n are the graphs with the maximal and minimal energies in the six-membered ring spiro chains. In the end, $Z_n \succ L_n \succ S_n$. ■

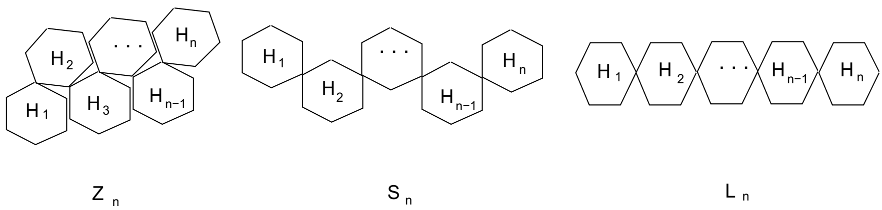

Figure 6: Z_n, L_n, S_n

Z_n, L_n, S_n are shown in Figure 6.

3. Polyphenyl chain

3.1. Definition. The *polyphenyl chain* is a graph consisting of N benzene rings $B_1, B_2, \ldots, B_N$ with the properties that for any $1 \leq k < j \leq N-1$ $(N \geq 1)$, B_k and B_j are linked by a cut edge if and only if $j = k+1$, and the common vertex of a benzene ring and a cut edge is denoted the vertex with degree three.

$H'(A, s)$ is the graph obtained by attaching the s-th vertex of P_n to the last benzene ring in the polyphenyl chain $A \in \mathbf{G}'_{i-1}$, $s = 1, 2, 3, \ldots n$ (see Figure 7).

Any element $G'_N \in \mathscr{G}'_{\mathscr{N}}$ can be obtained by linking a benzene ring to the last benzene ring of $G'_{N-1} \in \mathscr{G}'_{N-1}$. There are three non-isomorphic adding ways $G'_{N-1} \rightarrow [G'_{N-1}]_k = G'_N$, where $k = 1, 2, 3$ (see Figure 8). we call these three adding ways respectively: way-I, way-II, way-III.

Let A$\in \mathbf{G}'_{i-1}$, B $\in \mathbf{G}'_{N-i}$ and H_i be the benzene rings. B_i is linked to A by a single bond, denote by G'_i. If C is linked to G_i by way-k, we denote by $G'_N(i, k)$, where $G'_i \in \mathbf{G}'_i$, k=I, II, III (see Figure 9).

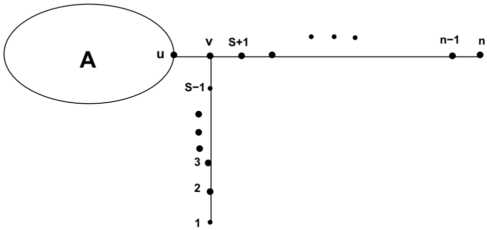

Figure 7: $H^{'}(A, s)$

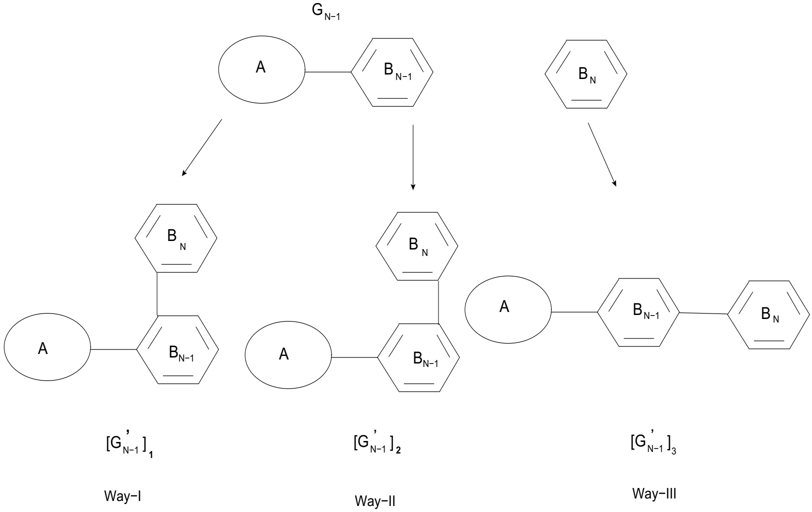

Figure 8: G_N'

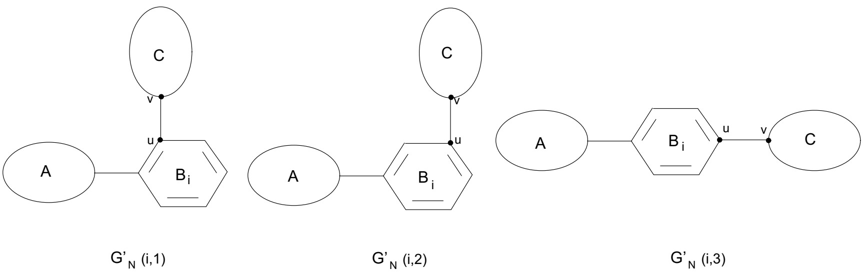

Figure 9: $G_N'(i, k)$

In particular, if every benzene ring in the polyphenyl chain is added by the way-I, then denote by Z_N; if every benzene ring in the polyphenyl chain is added by the way-II, then denote by S_N; if every benzene ring in the polyphenyl chain is added by the way-III, then denote by L_N. In this paper, we will prove that Z_N and S_N have the maximal and minimal energies in the set of polyphenyl chains.

3.2. Main result

Theorem 3.2.1. Let A be a polyphenyl chain with i benzene rings. Then $H'(A,1) \succ H'(A,3) \succ H'(A,5) \succ \cdots \succ H'(A,2k+1) \succ H'(A,2k) \succ H'(A,2k-2) \succ \cdots \succ H'(A,4) \succ H'(A,2)$.

Proof. It is obvious that a single bond can be viewed as an edge. Let uv be the edge connecting A and P_n in $H'(A,s)$ (see Figure 7). Compare the energies of two graphs, only to compare the corresponding coefficients of their characteristic polynomial by Lemma 2.2.3. On the other hand, by Lemma 2.2.2, we have

$$b_{2i}(H'(A,s)) = b_{2i}(H'(A,s) - uv) + b_{2i-2}(H'(A,s) - u - v) \ .$$

We can see that $H'(A,s) - uv = A \bigcup P_n$ for all $s = 1,2,3,\ldots,n$. So it suffices to consider $H'(A,s) - u - v$.

Clearly, $H'(A,s) - u - v = (A-u) \bigcup P_{s-1} \bigcup P_{n-s}$ by Lemma 5, we only see that $P_{s-1} \bigcup P_{n-s}$. By Lemma 2.2.4, we have $P_{n-1} \succ P_2 \bigcup P_{n-3} \succ P_4 \bigcup P_{n-5} \succ P_6 \bigcup P_{n-7} \succ \cdots \succ P_{2k} \bigcup P_{n-1-2k} \succ P_{2k+1} \bigcup P_{n-2k-2} \succ P_{2k-1} \bigcup P_{n-2k} \succ \cdots \succ P_3 \bigcup P_{n-4} \succ P_1 \bigcup P_{n-2}$. This leads to the result. ∎

Theorem 3.2.2. $G'_N(i,1) \succ G'_N(i,3) \succ G'_N(i,2)$.

Proof. Let the edge uv denote the bond connecting B_i and B_{i+1}, where u is the vertex in B_i, v is the vertex in first benzene ring of B (see Figure 8). Then

$$b_{2i}(G'_N(i,1)) = b_{2i}(G'_N(i,1) - uv) + b_{2i-2}(G'_N(i,1) - u - v)$$

for $k = 1,2,3$. Clearly, $G'_N(i,1) - uv$ are isomorphic for all $k = 1,2,3$.

It suffices to prove that

$$b_{2i-2}(G'_N(i,1) - u - v) \succ b_{2i-2}(G'_N(i,1) - u - v) \succ b_{2i-2}(G'_N(i,1) - u - v)$$

because

$$\begin{aligned} & G'_N(i,1) - u - v = H'(A,1) \bigcup (B - v), G'_N(i,3) - u - v \\ = \ & H'(A,3) \bigcup (B - v), G'_N(i,2) - u - v \\ = \ & H'(A,2) \bigcup (B - v) \ . \end{aligned}$$

By Theorem 3.2.1, we have $H'(A,1) \succ H'(A,3) \succ H'(A,2)$. This completes the proof. ■

Theorem 3.3.3. Among all the polyphenyl chains with N benzene rings, we have $Z_N \succ L_N \succ S_N$.

Proof. The proof is similar to that of Theorem 2.3.3. ■

Z_N, L_N, S_N are shown in the Figure 10.

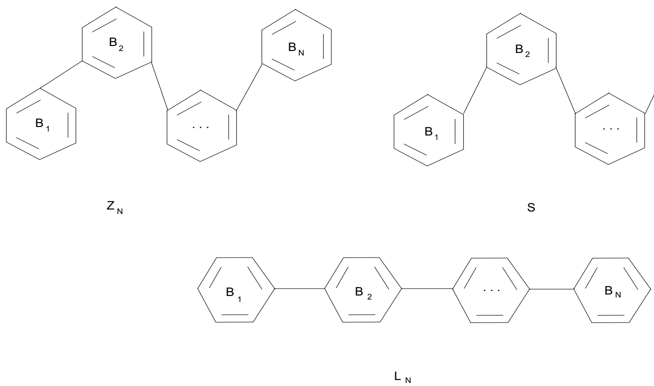

Figure 10: Z_N, L_N, S_N

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