Iranian J. Math. Chem. 10 (3) September (2019) 241 − 249

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

The Minimum Estrada Index of Spiro Compounds with k–Quadrangles

MOHAMMAD ALI IRANMANESH• AND RAZEIH NEJATI

Department of Mathematical Sciences, Yazd University, P. O. Box 89195−741, Yazd, I. R. Iran

ARTICLE INFO

Article History:

Received: 17 September 2018
Accepted: 6 March 2019
Published online: 30 September 2019
Academic Editor: Ali Reza Ashrafi

Keywords:

Spiro compounds
Estrada index
Symmetric Spiro

ABSTRACT

Let $G = (V, E)$ be a finite and simple graph with $\lambda_1, \lambda_2, \cdots, \lambda_n$ as its eigenvalues. The Estrada index of G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. A spiro compound is a chemical compound that presents a twisted structure of two or more rings, in which 2 or 3 rings are linked together by one common atom. In this paper, we will show that the symmetric and stable spiro compounds among all spiro compounds have the minimum Estrada index.

1. INTRODUCTION

Let $G = (V, E)$ be a simple graph, where by $V(G)$ and $E(G)$ denote the set of all vertices and edges of G, respectively. Let $A(G)$ be the adjacency matrix of G and $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of $A(G)$. The Estrada index of G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$ [7]. It has many applications in various fields such as network science, biochemistry and molecular graphs [6, 15, 16]. For theEstrada index of trees and an approximation of this graph invariant for cycles and paths, we refer to the papers [4, 10, 18, 8]. In [11, 12], the Estrada index of the cactus graphs in which every block is a triangle were computed.

Suppose $l \geq 0$ and $S_l(G) = \sum_{i=1}^{n} {\lambda_i}^l$ is the l-th spectral moment of G. It is well-known that this quantity is equal to the number of closed walks of length l in G and $S_0(G) = n$, $S_1(G) = c$, $S_2(G) = 2m$, $S_3(G) = 6d$, $S_4(G) = 2\sum_{i=1}^{n} {d_i}^2 - 2m + 8q$, where n, c, m, d, q denote the number of vertices, the number of loops, the number of edges, the number of triangles and the number of quadrangles of G, respectively. Moreover, we use the notation $d_i = d_i(G)$ to denote the degree of a the i-th vertex of G, i.e. v_i [3].

•Corresponding Author (Email address: iranmanesh@yazd.ac.ir)
DOI: 10.22052/ijmc.2019.149094.1392

Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, G_2, \dots, G_d$ as follows: Select a vertex of G_1, a vertex of G_2 and identify these two vertices and continue this manner inductively. More precisely, suppose that we have already constructed a graph from $G_1, G_2, \dots, G_i$, where $2 \le i \le d-1$. Then select a vertex in the already constructed graph (which may in particular be one of the selected vertices) and a vertex of G_{i+1}; and then identify these two vertices. We will briefly say that G is obtained by point attaching from $G_1, G_2, \dots, G_i$ and that G_is are the primary subgraphs of G [5].

A spiro compound is a chemical compound, typically an organic compound, that presents a twisted structure of two or more rings, in which 2 or 3 rings are linked together by one common atom The simplest spiro compounds are b_i-cyclic having just two rings, or have a b_i-cyclic portion as part of the larger ring system, in either case with the two rings connected through the defining single common atom. The one common atom connecting the participating rings distinguishes spiro compounds from other b_i-cyclic [17]. These compounds are classifying into two categories: symmetry and asymmetry. We consider the spiro compound with the even bonds in each ring and we will show that the spiro compounds with the least activation energy which are stable have the minimum Estrada index. For example, one of the smallest is shown in Figure 1.

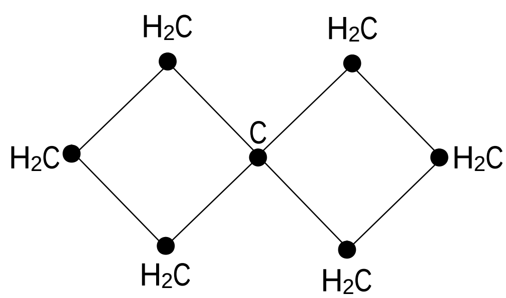
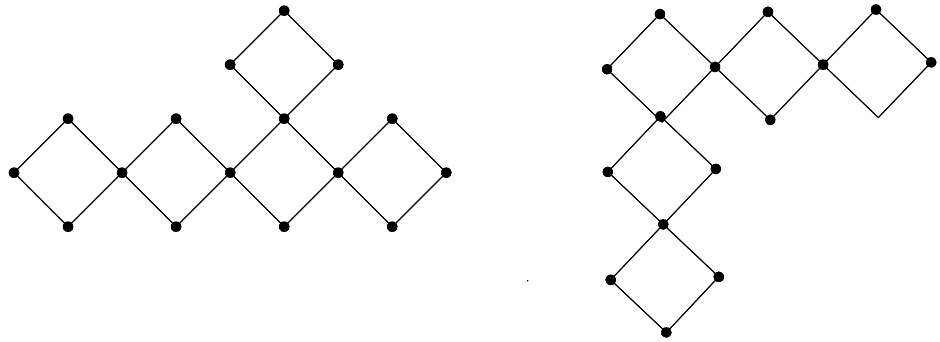
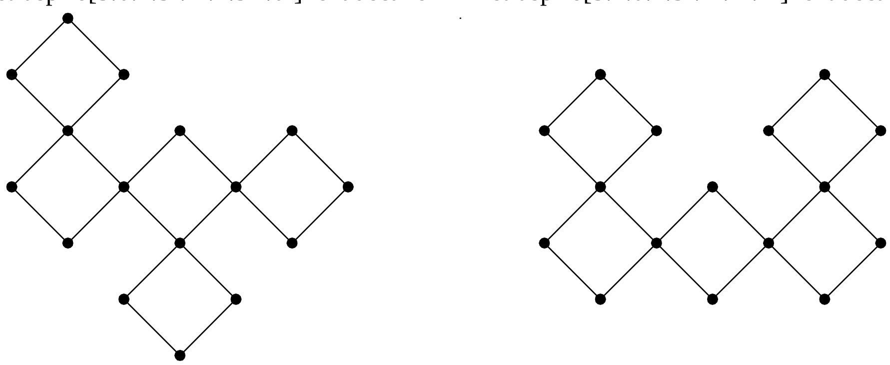


Figure 1. Spiro [3.3] heptane.

The spiro compounds isolated from plant and animal origins have important application in medical chemistry. The use of them as intermediates in synthesis, and the isolated characterization of new natural are particularly welcomed. Spiro compounds used as plasticizers (for example glycerinacetal cyclic ketons) in perfumery, intermediate products in the synthesis of epoxy, in producing medicine some spiro compounds are used as photochoromic materials. Spiro forms of lactones and oxazines are frequently used as leucodyes, frequently displaying chromism reversible change between their colorless and color form [14]. Examples of symmetry and asymmetry compounds with 5 quadrangles are shown in Figure 2.



Tetraspiro[3.0.1.3^{7}.1^{5}.1.3^{13}.0^{4}]hexadecane Tetraspiro[3.1.0.1.3^{9}.1^{7}.2^{6}.1^{4}]hexadecane



Tetraspiro[3.0.0.3^{6}.0.3^{10}.1^{5}.2^{4}]hexadecane Tetraspiro[3.0.1.0.3^{8}.2^{7}.1^{5}.2^{4}]hexadecane

Figure 2. Asymmetric and symmetric spiro compounds with 5 quadrangles.

Throughout this paper, $\Gamma(k)$ is a spiro compound which is symmetric and stable (stability occurs when a system is in its lowest energy state [13]) with k quadrangles, see Figure 3. We show that only $\Gamma(k)$ is possible to be the graph with minimum Estrada index among all spiro compounds with k quadrangles.

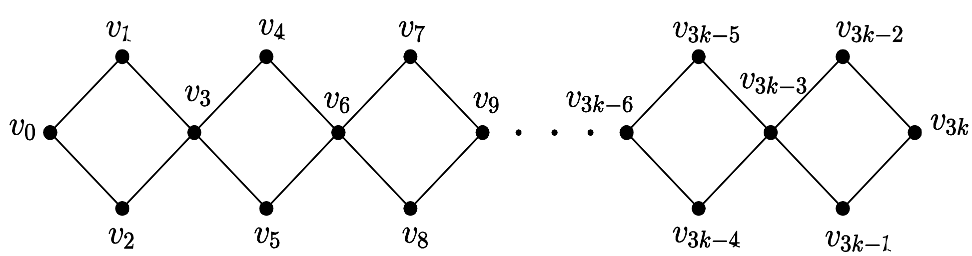


Figure 3. The graph $\Gamma(k)$.

An additional motivation for this fact is the following relation between $EE(G)$ and the spectral moment of G, when $l \geq 0$,

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i} = \sum_{i=1}^{n} \sum_{l=0}^{\infty} \frac{{\lambda_i}^l}{l!} = \sum_{l=0}^{\infty} \frac{S_l(G)}{l!}.$$

Theorem 1.1. Let G be a spiro compound with k quadrangles and $\Gamma(k)$ be the spiro compound which is shown in Figure 3. Then $EE(\Gamma(k)) < EE(G)$.

2. THE MINIMAL ESTRADA INDEX OF SPIRO COMPOUNDS WITH k QUADRANGLES

Let G_1 and G_2 be two graphs. If $S_l(G_1) \leq S_l(G_2)$ holds for all positive integer l, then $EE(G_1) \leq EE(G_2)$. Moreover, if the strict inequality $S_l(G_1) < (G_2)$ holds for at least one value $l_0 \geq 0$, then $EE(G_1) < EE(G_2)$. Recall that a sequence $a_0, a_1, \dots, a_n$ of numbers is said to be *unimodal* if for some $0 \leq i \leq n$ we have $a_0 \leq a_1 \leq \cdots \leq a_i \geq a_{i+1} \geq \cdots \geq a_n$ and this sequence is called *symmetric* if $a_i = a_{n-i}$ for $0 \leq i \leq n$ [2]. Thus a symmetric unimodal sequence $a_0, a_1, \dots, a_n$ has its maximum at the middle term (n is even) or middle two terms (n is odd). Let $S_l(3k, i)$ denote the number of closed walks of length l starting at the vertex v_i, $0 \leq i \leq 3$, in a given graph. It is well-known that the quantity $(A^l)_{i,j}$ represents the number of walks of length l from the i-th vertex v_i to the j-th vertex v_j [1]. Obviously, $(A^l)_{i,j} = (A^l)_{j,i}$ for undirected graphs.

Lemma 3.1 in [9] states that:

Lemma 2.1. *The map $\varphi: V(\Gamma(k)) \to V(\Gamma(k))$, given by $\varphi(v_i) = v_{k(c-1)-i}$ is an automorphism, when $0 \leq i \leq k(c-1) - i$.*

Let $c = 4$. Then we have:

Lemma 2.2. *The map $\varphi: V(\Gamma(k)) \to V(\Gamma(k))$, given by $\varphi(v_i) = v_{3k-i}$ is an automorphism, when $0 \leq i \leq 3k$.*

Proof. The proof is similar to Lemma 3.1 in [9]. ∎

As an immediate consequence, we have:

Corollally 2.3. *Let A be the adjacency matrix of $\Gamma(k)$. Then $(A^l)_{i,j} = (A^l)_{\varphi(i),\varphi(j)}$, where $0 \leq i, j \leq 3k$.*

Proof. This is an immediate consequence from definition of automorphism. ∎

Lemma 2.4. [See Lemma 3.3 in [9]]. *Let t, l be integers, $0 \leq t \leq c-2, l \geq c-1$ and $k \geq 2$, then*

$$S_l(k(c-1),t) \leq S_l\big(k(c-1),t+(c-1)\big) \leq \cdots$$
$$\leq S_l\left(k(c-1),t+\left(\left\lceil\frac{k}{2}\right\rceil-1\right)(c-1)\right)$$
$$\leq S_l\left(k(c-1),t+\left\lceil\frac{k}{2}\right\rceil(c-1)\right).$$

For $l \geq \frac{k}{2}$, the strict inequality hold.

In what follows, we consider the case of $c = 4$.

Lemma 2.5. *Let $\Gamma(k)$ be the spiro compound which is shown in Figure* 3. *Then for any integer t with $0 \leq 3t \leq \frac{3k}{2}$, $l > 3$ and $3k \geq 6$,*

$$\begin{cases} S_l(3k,0) \leq \cdots \leq S_l(3k,3t) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-3\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil\right), \ if \left\lceil\frac{3k}{2}\right\rceil \equiv 0(mod\ 3) \\ S_l(3k,0) \leq \cdots \leq S_l(3k,3t) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-4\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-1\right), if \left\lceil\frac{3k}{2}\right\rceil \equiv 1(mod\ 3), \\ S_l(3k,0) \leq \cdots \leq S_l(3k,3t) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-5\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-2\right), if \left\lceil\frac{3k}{2}\right\rceil \equiv 2(mod\ 3) \end{cases}$$

and the strict inequalities hold for sufficiently large l.

Lemma 2.6. *Let $\Gamma(k)$ be the spiro compound which is shown in Figure* 3. *Then for any integer t with $0 \leq 3t + 1.3t + 2 \leq \frac{[3k]}{2}$, $l > 3$ and $3k \geq 6$,*

$$\begin{cases} S_l(3k,1) \leq \cdots \leq S_l(3k,3t+1) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-2\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil+1\right) & \left\lceil\frac{3k}{2}\right\rceil \equiv 0(mod\ 3) \\ S_l(3k,1) \leq \cdots \leq S_l(3k,3t+1) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-3\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil\right) & \left\lceil\frac{3k}{2}\right\rceil \equiv 1(mod\ 3), \\ S_l(3k,1) \leq \cdots \leq S_l(3k,3t+1) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-4\right) \leq S_l\left(3k.\left\lceil\frac{3k}{2}\right\rceil-1\right) & \left\lceil\frac{3k}{2}\right\rceil \equiv 2(mod\ 3) \end{cases}$$

and

$$\begin{cases} S_l(3k,2) \leq \cdots \leq S_l(3k,3t+2) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-4\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-1\right) & \left\lceil\frac{3k}{2}\right\rceil \equiv 0(mod\ 3) \\ S_l(3k,2) \leq \cdots \leq S_l(3k,3t+2) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-2\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil+1\right) & \left\lceil\frac{3k}{2}\right\rceil \equiv 1(mod\ 3), \\ S_l(3k,2) \leq \cdots \leq S_l(3k,3t+2) \leq \cdots \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil-3\right) \leq S_l\left(3k,\left\lceil\frac{3k}{2}\right\rceil\right) & \left\lceil\frac{3k}{2}\right\rceil \equiv 2(mod\ 3) \end{cases}$$

and the strict inequalities hold for $l \geq \left\lceil\frac{3k}{2}\right\rceil + 1$.

Suppose G^1 is a spiro compound with k quadrangles different from $\Gamma(k)$. For $k_2 < k$, let $k_2 \coloneqq \max\{u: \Gamma(u)\ is\ a\ subgraph\ of\ G^1\}$, B_0 be the set of all subgraphs which are connected with the vertices that their indices are congruent to $0 \pmod 3$ and $\Gamma(k_2)$ has b_i quadrangles, $0 \leq i \leq k - k_2$. Let $k_1 \coloneqq \max\{b_i: 0 \leq i \leq k - k_2\}$, G be a spiro compound with k_1 quadrangles, $\alpha \in V(G)$ and $G(\left\lceil\frac{k_2}{2}\right\rceil, \left\lceil\frac{k_2}{2}\right\rceil)$ be the spiro obtained from G by attaching two spiros $\Gamma(\left\lfloor\frac{k_2}{2}\right\rfloor)$ and $\Gamma(\left\lceil\frac{k_2}{2}\right\rceil)$ at α. Moreover, we assume that $M_l(G\left(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil\right); \alpha)$ and $M_l(G\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1. \left\lceil\frac{k_2}{2}\right\rceil - 1\right); \alpha)$ are the set of all $(\alpha. \alpha)$-walks of length l in $G\left(\left\lfloor\frac{k_2}{2}\right\rfloor. \left\lceil\frac{k_2}{2}\right\rceil\right)$ and $G\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1. \left\lceil\frac{k_2}{2}\right\rceil - 1\right)$ starting and ending at the edges or only one edge in G, respectively. Similarly,

$$M'_l(G\left(\left\lfloor\frac{k_2}{2}\right\rfloor. \left\lceil\frac{k_2}{2}\right\rceil\right); \alpha) \text{ and } M'_l(G\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1. \left\lceil\frac{k_2}{2}\right\rceil - 1\right); \alpha)$$

are the set of all $(\alpha. \alpha)$-walks of length l in $G\left(\left\lfloor\frac{k_2}{2}\right\rfloor. \left\lceil\frac{k_2}{2}\right\rceil\right)$ and $G\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1. \left\lceil\frac{k_2}{2}\right\rceil - 1\right)$ starting and ending at the edges or only one edge in

$$\Gamma(\left\lfloor\frac{k_2}{2}\right\rfloor) \cup \Gamma(\left\lceil\frac{k_2}{2}\right\rceil) \text{and } \Gamma(\left\lfloor\frac{k_2}{2}\right\rfloor + 1) \cup \Gamma(\left\lceil\frac{k_2}{2}\right\rceil - 1),$$

respectively. Finally, define$G\left(\left\lfloor\frac{k_2}{2}\right\rfloor. \left\lceil\frac{k_2}{2}\right\rceil\right) \coloneqq G(1)$ and $G\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1. \left\lceil\frac{k_2}{2}\right\rceil - 1\right) \coloneqq G(2)$.

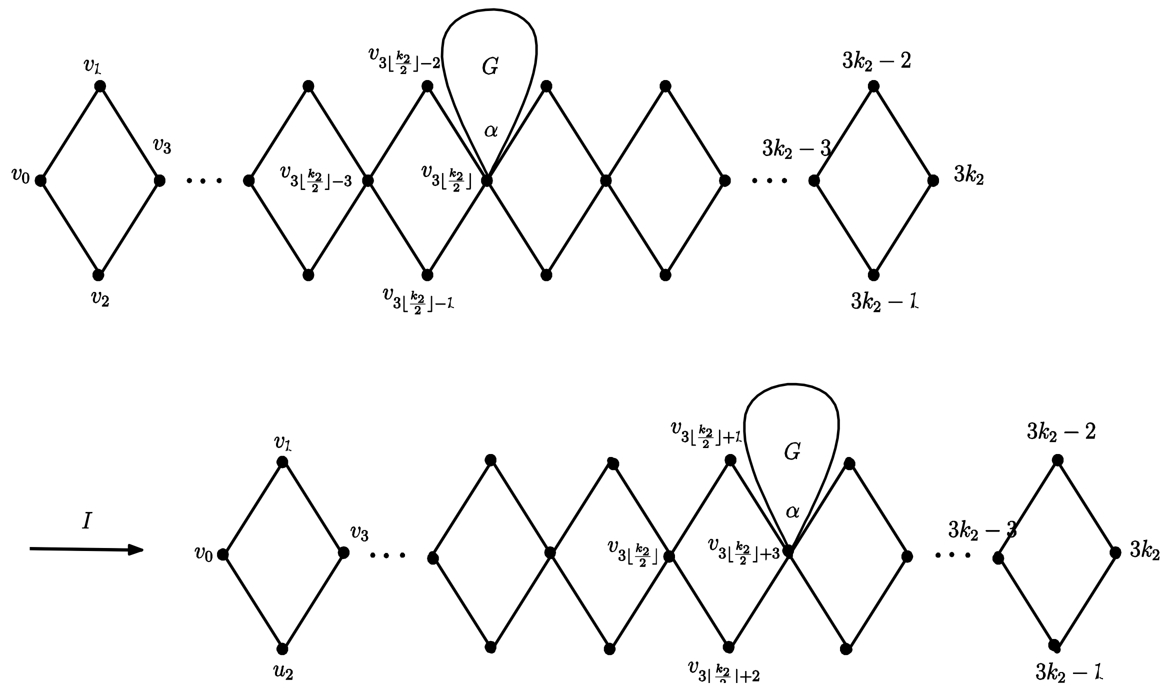


Figure 4. Transformation I.

Suppose that G^2 is a spiro compound with k quadrangles different from $\Gamma(k)$. For $k_2 < k$, let $k_2 \coloneqq \max\{u: \Gamma(u) \text{ is a subgraph of } G^2\}$, B_1 be the set of all subgraphs that are connected to the vertices in which their indices are congruent to 1 or $2 \pmod 3$ and $\Gamma(k_2)$ has b_i quadrangles, $0 \le i \le k - k_2$. Let $k_1 \coloneqq \max\{b_i: 0 \le \mathrm{i} \le k - k_2\}$, G be a spiro compound with k_1 quadrangles, $\delta \in V(G)$ and $G'(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil)$ be the spiro obtained from G' by attaching two spiros $\Gamma(\left\lfloor\frac{k_2}{2}\right\rfloor)$ and $\Gamma(\left\lceil\frac{k_2}{2}\right\rceil)$ at δ. Let $N_l(G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil\right); \delta)$ and

$N_l(G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1.\left\lceil\frac{k_2}{2}\right\rceil - 1\right); \delta)$ be the set of all $(\alpha.\alpha)$-walks of length l in $G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil\right)$ and $G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1, \left\lceil\frac{k_2}{2}\right\rceil - 1\right)$ starting and ending at the edges or only one edge in G, respectively. Moreover, we assume that

$$N'_l(G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil\right); \delta) \text{ and } N'_l(G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1, \left\lceil\frac{k_2}{2}\right\rceil - 1\right); \delta)$$

are the set of all $(\alpha.\alpha)$-walks of length l in

$$G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil\right) \text{ and } G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1, \left\lceil\frac{k_2}{2}\right\rceil - 1\right)$$

starting and ending at the edges or only one edge in

$$\Gamma(\left\lfloor\frac{k_2}{2}\right\rfloor) \cup \Gamma(\left\lceil\frac{k_2}{2}\right\rceil) \text{ and } \Gamma\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1\right) \cup \Gamma\left(\left\lceil\frac{k_2}{2}\right\rceil - 1\right),$$

respectively. Finally, define $G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor, \left\lceil\frac{k_2}{2}\right\rceil\right) \coloneqq G'(1)$ and $G'\left(\left\lfloor\frac{k_2}{2}\right\rfloor + 1, \left\lceil\frac{k_2}{2}\right\rceil - 1\right) \coloneqq G'(2)$. By applying Theorem 4.2 in [9], we have the following theorems:

Theorem 2.7. *Let l be a positive integer and $\left\lfloor\frac{k_2}{2}\right\rfloor \geq 1$. Then*

i. $|M_l(G(2)); \alpha| \leq |M_l(G(1)); \alpha|$.
ii. $|M'_l(G(2)); \alpha| \leq |M'_l(G(1)); \alpha|$.
iii. $S_l(G(2)) \leq S_l(G(1))$.

The strict inequality holds when $l \geq \left\lceil\frac{3k_2}{2}\right\rceil$.

Theorem 2.8. *Let l be a positive integer and $\left\lfloor\frac{k_2}{2}\right\rfloor \geq 1$. Then*

i. $|N_l(G'(2)); \delta| \leq |N_l(G'(1)); \delta|$.
ii. $|N'_l(G'(2)); \delta| \leq |N'_l(G'(1)); \delta|$.
iii. $S_l(G'(2)) \leq S_l(G'(1))$.

The strict inequality holds when $l \geq \left\lceil\frac{3k_2}{2}\right\rceil$.

Corollary 2.9. $EE(G(2)) < EE(G(1))$.

Proof. By Theorem 2.7, $EE(G(2)) = \sum_{l\geq 0}\frac{S_l(G(2))}{l!} < \sum_{l\geq 0}\frac{S_l(G(1))}{l!} = EE(G(1))$, proving the result. ∎

Corollary 2.10. $EE(G'(2)) < EE(G'(1))$.

Proof. By Theorem 2.8, $EE(G'(2)) = \sum_{l\geq 0}\frac{S_l(G'(2))}{l!} < \sum_{l\geq 0}\frac{S_l(G'(1))}{l!} = EE(G'(1))$, proving the result. ∎

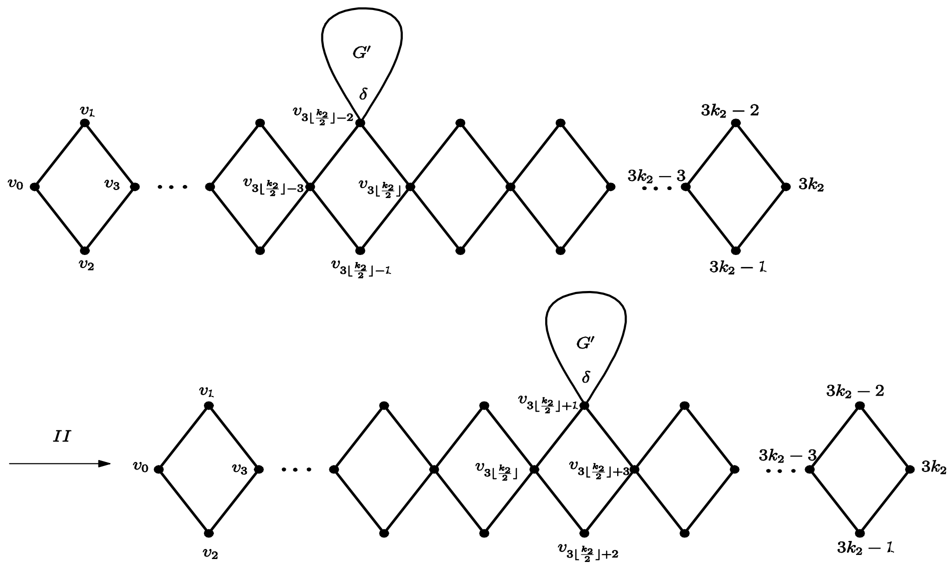


Figure 5. Transformation II.

Let G be a spiro compound with k quadrangles and maximum degree Δ at the vertex u containing the subgraphs $G_1, G_2, \ldots, G_{\Delta/2}$ with exactly one common vertex at u. Using transformations see [18], G_is can be transformed into $\Gamma(k_i)$s. By these transformations, G changes into G^*. Each application of transformations strictly decreases its Estrada index and so $EE(G^*) < EE(G)$. Next by repeatedly application of the transformation I, G^* can be changed into the graph $\Gamma(k)$. So we have the following result:

Theorem 2.11. *Let G be a spiro compound with k quadrangles and $\Gamma(k)$ be the spiro compound as it shown in Figure* 3. *Then* $EE(\Gamma(k) < EE(G)$.

REFERENCES

1. N. Biggs, *Algebraic Graph Theory*, Cambridge University Press, Cambridge, 1993.
2. G. Boros and V. H. Moll, A criterion for unimodality, *Electron. J. Combin.* **6** (1) (1999), #R10.
3. D. Cvetkovic, M. Doob and H. Sachs, *Spectra of Graphs, Theory and Applications*, Academic Press, New York, 1980.
4. H. Deng, A proof of a conjecture on the Estrada index, *MATCH Commun. Math. Comput. Chem.* **62** (3) (2009) 599–606.
5. E. Deutsch and S. Klavžar, Computing Hosoya polynomials of graphs from primary subgraphs, *MATCH Commun. Math. Comput. Chem.* **70** (2) (2013) 627–644.

6. E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (5−6) (2000) 713–718.
7. E. Estrada, Characterization of the folding degree of proteins, *Bioinformatics* **18** (5) (2002) 697–704.
8. I. Gutman and A. Graovac, Estrada index of cycles and paths, *Chem. Phys. Lett.* **436** (1−3) (2007) 294–296.
9. M. A. Iranmanesh and R. Nejati, On the Estrada index of point attaching strictk-quasi tree graphs, *Kragujevac J. Math.* **44** (2) (2020) 165–179.
10. J. Li, X. Li and L. Wang, The minimal Estrada index of trees with two maximum degree vertices, *MATCH Commun. Math.Comput. Chem*. **64** (2010) 799–810.
11. F. Li, L. Wei, J. Cao, F. Hu and H. Zhao, On the maximum Estrada index of 3-uniform linear hypertrees, *Scientific World J.* **8** (2014) 1–8.
12. F. Li, L. Wei, H. Zhao, F. Hu and X. Ma, On the Estrada index of cactus graphs, *Discrete Appl. Math.* **203** (2016) 94–105.
13. A. D. McNaught, *Compendium of Chemical Terminology*, Blackwell Science Publication, Oxford, 1997.
14. R. Rios, Enantioselective methodologies for the synthesis of spiro compounds, *Chem. Soc. Rev*. **41** (3) (2012) 1060–1074.
15. Y. Shang, Random lifts of graphs: network robustness based on the Estrada index, *Appl. Math. E-Notes* **12** (2012) 53–61.
16. Y. Shang, Biased edge failure in scale-free networks based on natural connectivity, *Indian J. Phys*. **86** (6) (2012) 485–488.
17. A. Von Zelewsky, *Stereochemistry of Coordination Compounds*, John Wiley & Sons, Chichester, 1996.
18. J. Zhang, B. Zhou and J. Li, On Estrada index of trees, *Linear Algebra Appl*. **434** (1) (2011) 215–223.