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Topological indices of splitting graph of special case of hexagonal system

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Abstract:A topological index is a numeric number that helps to find the characteristics of a compounds. There are many applications of graph theory. In this paper we compute first and second Zagreb indices, Randi´c index, sum-connectivity index, harmonic index, inverse sum indeg index, modified first and second Zagreb indices and first and second hyper-Zagreb indices of the Splitting graph of the special case of hexagonal system.

Keywords: Molecular graph,topological indices, hexagonal system.

I. Introduction

Topological indices help for the quantitative structures property relationship (QSPR) and quantitative structure activity relationship (QSAR).

Let G be a simple graph, with vertex set V(G) and edge set E(G).The degree $d_u$of a vertex uis the number of edges that are incident to it.

Since 1947 many number of topological indices have been found. One of the oldest and well known topological indices is the first and second Zagreb indices, was first introduced by Gutman et al. in 1972 [3], and it is defined as

$$M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$$

and $$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$$

The connectivity index introduced in 1975 by Milan Randi´c [4], is defined as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Recently, another variant of the Randi´c connectivity index called the sum-connectivity index was introduced by B. Zhou and N. Trinajsti´c [5] in 2008. It is defined as,

$$X(G) = \sum_{uv\in E(G)} \frac{1}{d_u + d_v}$$

In 2014 Jianxi Li and Chee Shiu introduced a new variant of the Randi´c index named the Harmonic index which first appeared in [6] called the harmonic index H (G) is defined as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v}$$

Discrete Adriatic indices have been defined by Vukičević and Gašperov in 2010 . One among such indices is the inverse sum indeg index, [7] and is defined as

$$ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u+d_v}$$

A. Milicevi, S. Nikoli, N. Trinajstic, introduced in 2004 the modified first and second Zagreb indices [8], and are respectively defined as

$$^{m}M_1(G) = \sum_{u\in V(G)} \frac{1}{d_G(u)^2}$$

$$^{m}M_2(G) = \sum_{uv\in E(G)} \frac{1}{d_G(u)d_G(v)}$$

In 2013 [9], Shirdel et al. introduced the first hyper-Zagreb index of a graph G, which is defined as

$$HM_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]^2$$

In [10], the second hyper-Zagreb index of a graph G is defined as

$$HM_2(G) = \sum_{uv\in E(G)} [d_G(u)d_G(v)]^2$$

II. HEXAGONAL SYSTEM

A hexagonal system is defined as a 2-connected plane graph in which every interior face is bounded by a regular hexagon of unit length 1. A hexagonal system H is said to be Catacondensed if it does not possess internal vertices, otherwise H is said to be Pericondensed. A hexagonal chain is a Catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. Some examples of hexagonal chains can be found in Fig. 1.

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One can easily see that, H_{n+1} is a hexagonal chain obtained from H_n by attaching $n+1$ hexagons.

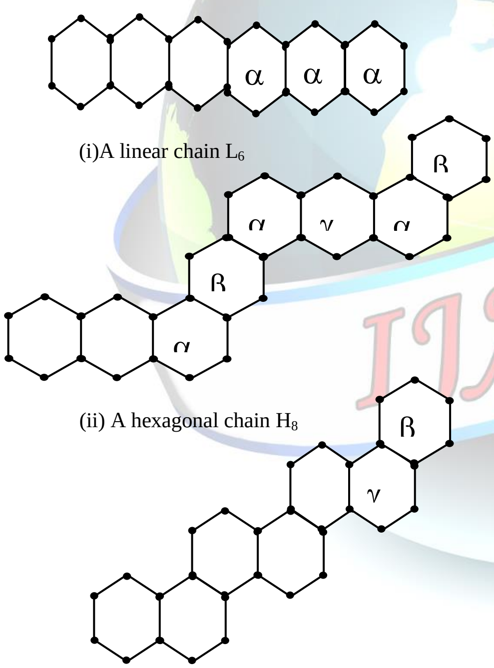
Based on this we define three types of fusion for attaching a new hexagon h_{n+1} to a hexagonal chain H_n with n hexagons $h_1, h_2, h_3, \ldots . h_n$:

(i) If h_{n+1} is on the line l, it is called $\propto -$type fusing;

(ii) If h_{n+1} is on the left-hand side of l, it is called $\beta -$ type fusing;

(iii) If h_{n+1} is on the right-hand side of l, it is called $\gamma -$ type fusing

where l is the direct line from the center of h_{n-1} to the center of h_n . Any hexagonal chain $H_n (n \geq 2)$ can be obtained fromH_2 by a stepwise fusion of new hexagons, and at each step a$\theta -$type fusion is selected, where $\in \{\alpha, \beta, \gamma\}$. Below are examples of the above said three types of fusing in Hexagonal system.



(i)A linear chain L_6

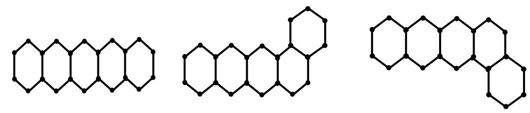
(ii) A hexagonal chain H_8

(iii) A Zig-zag chain Z_7

Fig 2.1. Single hexagonal chains with different types of fusions.

III. MAIN RESULTS

In this chapter we compute topological indices of on splitting graph of special case of hexagonal system. That is we are going to study the topological indices of Linear chain with $\propto, \beta$ andγ types of fusing .Fig 2 shows the Linear chain with $\propto -$type, $\beta -$ type and $\gamma -$ type fusing of length 5 which is denoted as $L_5(\alpha, \alpha)$, $L_5(\alpha, \beta)$ and $L_5(\alpha, \gamma)$.



$L_5(\alpha, \alpha)$ $L_5(\alpha, \beta)$ $L_5(\alpha, \gamma)$

Fig 3.1. Linear chainL_5 with α, β, γ type fusing

Defenition 3.1 [14].

The Splitting graph S(G) of graph G is the graph where for each point v of a graph G, take a new point v′and join v′ to all points of G adjacent tov.

The following diagram shows the linear chain $L_3(\alpha, \alpha)$ and its Splitting graph $S[\, L_3(\alpha, \alpha)]$

$L_3(\alpha, \alpha)$ $S[\, L_3(\alpha, \alpha)]$

Fig 3.2. Linear chainL_3 with $\alpha -$ type fusing and its Splitting graph

Theorem 3.1:

If $S\big(\, L_n(\alpha, \alpha)\big)$ is a linear chain with $\alpha -$ type fusing , then

(i) $M_1(G) = 5(26n + 13)$

$M_2(G) = 24(11n - 3)$

$$\text{(ii)} R(G) = \frac{1}{6}\begin{bmatrix} 3\big(3+6\sqrt{2}\big) + (n-1) \\ \big(1 + 2\sqrt{6} + 8\sqrt{3}\; 2\sqrt{2}\big) \end{bmatrix}$$

$$\text{(iii)} X(G) = \frac{1}{1260}\big(3465 + 2239(n-1)\big)$$

$$\text{(iv)} H(G) = \frac{1}{630}\big(3465 + 2239(n-1)\big)$$

$$\text{(v)} ISI(G) = \frac{1}{35}\big(980 + 1031(n-1)\big)$$

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$$\text{(vi)}\,{}^{m}M_1(G)=\frac{1}{144}[90(n+2)+40(n-1)]$$

$$ {}^{m}M_2(G)=\frac{1}{288}[540+280(n-1)]$$

$$\text{(vii)}HM_1(G)=816+1158(n-1)$$

$$HM_2(G)=2304+5400(n-1)$$

Proof

Let the graph $G=S(L_n(\alpha,\alpha))$ is a linear chain with $\alpha-$ type fusing as shown in the following diagram

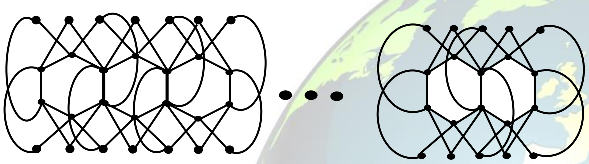

Fig 3.3. Splitting graph of Linear chain L_n with $\alpha-$type fusing

In $S(L_n(\alpha,\alpha))$ we see that $\left|V\left(S(L_n(\alpha,\alpha))\right)\right|=4(2n+1)$ and $\left|E\left(S(L_n(\alpha,\alpha))\right)\right|=3(5n+1)$. There are 4 types of vertices with degree namely $V_2, V_3, V_4,$ and V_6. Hence we have

$$\left|V_2\left(S(L_n(\alpha,\alpha))\right)\right|=\left|V_4\left(S(L_n(\alpha,\alpha))\right)\right|=2(n+2)$$

and

$$\left|V_3\left(S(L_n(\alpha,\alpha))\right)\right|=\left|V_6\left(S(L_n(\alpha,\alpha))\right)\right|=2(n-1).$$

Also the edges with degrees of end vertices in $S(L_n(\alpha,\alpha))$ is as follows:

There are $(n-1)$ edges with degrees of end vertices(6,6); 6 edges with degrees of end vertices(4,4); $4(n-1)$ edges with degrees of end vertices(4,6); 12 edges with degrees of end vertices(2,4); $4(n-1)$ edges with degrees of end vertices(2,6); $4(n-1)$ edges with degrees of end vertices(3,4); $2(n-1)$ edges with degrees of end vertices(3,6). Hence

$$\text{(i)}M_1(G)=\sum\nolimits_{uv\in E(G)}[d_G(u)+d_G(v)]$$

$$=(n-1)(6+6)+6(4+4)+4(n-1)(4+6)+12(2+4)+4(n-1)(2+6)+4(n-1)(4+3)+2(n-1)(3+6)=5(26n+13)$$

$$M_2(G)=\sum_{uv\in E(G)} d_G(u)d_G(v)$$

$$=(n-1)(6\times 6)+6(4\times 4)+4(n-1)(4\times 6)+12(2\times 4)+4(n-1)(2\times 6)+4(n-1)(4\times 3)+2(n-1)(3\times 6)=24(11n-3)$$

$$\text{(ii)}R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}$$

$$=\frac{(n-1)}{\sqrt{6\times 6}}+\frac{6}{\sqrt{4\times 4}}+\frac{4(n-1)}{\sqrt{4\times 6}}+\frac{12}{\sqrt{2\times 4}}+\frac{4(n-1)}{\sqrt{2\times 6}}+\frac{4(n-1)}{\sqrt{3\times 4}}+\frac{2(n-1)}{\sqrt{3\times 6}}=\frac{1}{6}\left[\begin{array}{c}3(3+6\sqrt{2})+(n-1)\\(1+2\sqrt{6}+8\sqrt{3}+2\sqrt{2})\end{array}\right]$$

$$\text{(iii)}X(G)=\sum_{uv\in E(G)}\frac{1}{d_u+d_v}$$

$$=\frac{(n-1)}{6+6}+\frac{6}{4+4}+\frac{4(n-1)}{4+6}+\frac{12}{2+4}+\frac{4(n-1)}{2+6}+\frac{4(n-1)}{3+4}+\frac{2(n-1)}{3+6}=\frac{1}{1260}\left(3465+2239(n-1)\right)$$

$$\text{(iv)}H(G)=\sum_{uv\in E(G)}\frac{2}{d_u+d_v}$$

$$\frac{2(n-1)}{6+6}+\frac{2(6)}{4+4}+\frac{2\left(4(n-1)\right)}{4+6}+\frac{2(12)}{2+4}+\frac{2\left(4(n-1)\right)}{2+6}+\frac{2\left(4(n-1)\right)}{3+4}+\frac{2\left(2(n-1)\right)}{3+6}=\frac{1}{630}\left(3465+2239(n-1)\right)$$

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$$(v)ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$
$$= (n-1)\left(\frac{6\times 6}{6+6}\right) + 6\left(\frac{4\times 4}{4+4}\right)$$
$$+4(n-1)\left(\frac{4\times 6}{4+6}\right) + 12\left(\frac{2\times 4}{2+4}\right)$$
$$+4(n-1)\left(\frac{2\times 6}{2+6}\right) + 4(n-1)\left(\frac{3\times 4}{3+4}\right)$$
$$+2(n-1)\left(\frac{3\times 6}{3+6}\right) = \frac{1}{35}\left(980 + 1031(n-1)\right)$$

$$(vi)\,{}^{m}M_1(G) = \sum_{u\in V(G)} \frac{1}{d_G(u)^2}$$
$$= 2(n+2)\left(\frac{1}{2^2}\right) + 2(n+2)\left(\frac{1}{4^2}\right)$$
$$+2(n-1)\left(\frac{1}{3^2}\right) + 2(n-1)\left(\frac{1}{6^2}\right)$$
$$= \frac{1}{144}[90(n+2) + 40(n-1)]$$

$${}^{m}M_2(G) = \sum_{uv\in E(G)} \frac{1}{d_G(u)d_G(v)}$$
$$= (n-1)\left(\frac{1}{6\times 6}\right) + 6\left(\frac{1}{4\times 4}\right)$$
$$+4(n-1)\left(\frac{1}{4\times 6}\right) + 12\left(\frac{1}{2\times 4}\right)$$
$$+4(n-1)\left(\frac{1}{2\times 6}\right) + 4(n-1)\left(\frac{1}{4\times 3}\right)$$
$$+2(n-1)\left(\frac{1}{3\times 6}\right) = \frac{1}{288}[540 + 280(n-1)]$$

$$(vii)HM_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]^2$$
$$= (n-1)(6+6)^2 + 6(4+4)^2 +$$
$$4(n-1)(4+6)^2 + 12(2+4)^2 +$$
$$4(n-1)(2+6)^2 + 4(n-1)(3+4)^2 +$$
$$2(n-1)(3+6)^2 = 816 + 1158(n-1)$$

$$HM_2(G) = \sum_{uv\in E(G)} [d_G(u)d_G(v)]^2$$
$$= (n-1)(6\times 6)^2 + 6(4\times 4)^2 +$$
$$4(n-1)(4\times 6)^2 + 12(2\times 4)^2 +$$
$$4(n-1)(2\times 6)^2 + 4(n-1)(3\times 4)^2 +$$
$$2(n-1)(3\times 6)^2 = 2304 + 5400(n-1)$$

Example 3.1:
Consider the graph $G = S(L_4(\alpha,\alpha))$. Then we have, $\left|V\left(S(L_4(\alpha,\alpha))\right)\right| = 36$; $\left|E\left(S(L_4(\alpha,\alpha))\right)\right| = 63$.Here $|V_2| = |V_4| = 12$ $|V_3| = |V_6| = 6$. Also there are 3 edges with degrees of end vertices(6,6); 6 edges with degrees of end vertices(4,4);12 edges with degrees of end vertices(4,6); 12 edges with degrees of end vertices(2,4);12 edges with degrees of end vertices(2,6);12 edges with degrees of end vertices(3,4);6 edges with degrees of end vertices(3,6). Hence

$$(i)M_1(G) = 510$$
$$M_2(G) = 984$$
$$(ii)R(G) = 18.535$$
$$(iii)X(G) = 7.93$$
$$(iv)H(G) = 16.162$$
$$(v)ISI(G) = 116.37$$
$$(vi)\,{}^{m}M_1(G) = 4.583$$
$${}^{m}M_2(G) = 4.792$$
$$(vii)HM_1(G) = 4290$$
$$HM_2(G) = 18504$$

Theorem 3.2:
If $S(L_n(\alpha,\beta))$ is a linear chain with $\beta-$type fusing and $S(L_n(\alpha,\gamma))$ with $\gamma-$type fusing then we see that both the chains are symmetric and hence $S(L_n(\alpha,\beta)) = S(L_n(\alpha,\gamma))$.Hence

$$(i)M_1(G) = 130n - 10$$

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$$M_2(G) = 8(33n - 8)$$

$$(ii) R(G) = \frac{1}{24\sqrt{6}}\left[6\left(7\sqrt{6} + 28\sqrt{3} - 12 - 24\sqrt{2}\right) + 4n\left(12 + \sqrt{6} + 24\sqrt{2}\right)\right]$$

$$(iii) X(G) = \frac{1}{3780}(3178980 + 6717n)$$

$$(iv) H(G) = \frac{1}{1890}(1589490 + 6717n)$$

$$(v) ISI(G) = \frac{1}{105}(3093n - 107)$$

$$(vi) {}^{m}M_1(G) = \frac{1}{144}[90(n+2) + 40(n-1)]$$

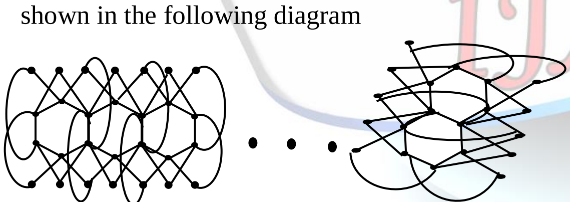
$${}^{m}M_2(G) = \frac{1}{576}[540 + 560n]$$

$$(vii) HM_1(G) = 1158n - 326$$

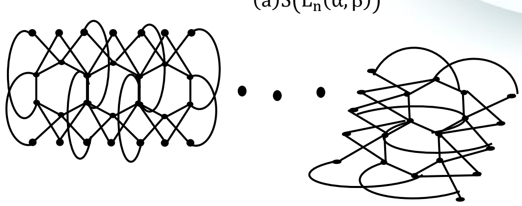
$$HM_2(G) = 5400n - 2496$$

Proof

Let the graph $G = S(L_n(\alpha,\beta))$ is a linear chain with $\beta -$ type fusing and $S(L_n(\alpha,\gamma))$ with $\gamma -$ type fusing as shown in the following diagram



(a) $S(L_n(\alpha,\beta))$



(b) $S(L_n(\alpha,\gamma))$

Fig 3.4. Splitting graph of Linear chain L_n with $\beta -$ type fusing and $\gamma -$ type fusing

In $S(L_n(\alpha,\beta))$ and $S(L_n(\alpha,\gamma))$ we see that $|V| = 4(2n+1)$ and $|E| = 3(5n+1)$. There are 4 types of vertices with degree namely $V_2, V_3, V_4,$ and V_6. Hence we have $|V_2| = |V_4| = 2(n+2)$
And $|V_3| = |V_6| = 2(n-1)$.

Also the edges with degrees of end vertices in $S(L_n(\alpha,\beta)) = S(L_n(\alpha,\gamma))$ is as follows:
There are n edges with degrees of end vertices(6,6); 7 edges with degrees of end vertices(4,4);($4n-6$) edges with degrees of end vertices(4,6); 14 edges with degrees of end vertices(2,4);($4n-6$) edges with degrees of end vertices(2,6); ($4n-6$) edges with degrees of end vertices(3,4); 2n edges with degrees of end vertices(3,6). Hence

$$(i) M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$$
$$= n(6+6) + 7(4+4) + (4n-6)(4+6) + 14(2+4) + (4n-6)(2+6) + (4n-6)(4+3) + 2n(3+6) = 130n - 10$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u) d_G(v)$$
$$= n(6\times 6) + 7(4\times 4) + (4n-6)(4\times 6) + 14(2\times 4) + (4n-6)(2\times 6) + (4n-6)(4\times 3) + 2n(3\times 6) = 8(33n-8)$$

$$(ii) R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$
$$= \frac{n}{\sqrt{6\times 6}} + \frac{7}{\sqrt{4\times 4}} + \frac{(4n-6)}{\sqrt{4\times 6}} + \frac{14}{\sqrt{2\times 4}} + \frac{(4n-6)}{\sqrt{2\times 6}} + \frac{(4n-6)}{\sqrt{3\times 4}} + \frac{2n}{\sqrt{3\times 6}} =$$
$$= \frac{1}{24\sqrt{6}}\left[6\left(7\sqrt{6} + 28\sqrt{3} - 12 - 24\sqrt{2}\right) + 4n\left(12 + \sqrt{6} + 24\sqrt{2}\right)\right]$$

$$(iii) X(G) = \sum_{uv\in E(G)} \frac{1}{d_u + d_v}$$

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$$= \frac{n}{6+6} + \frac{7}{4+4} + \frac{(4n-6)}{4+6} + \frac{14}{2+4} + \frac{(4n-6)}{2+6} + \frac{(4n-6)}{3+4} + \frac{2n}{3+6}$$

$$= \frac{1}{3780}(3178980 + 6717n)$$

$$(iv) H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

$$\frac{2n}{6+6} + \frac{2(7)}{4+4} + \frac{2((4n-6))}{4+6} + \frac{2(14)}{2+4} + \frac{2((4n-6))}{2+6} + \frac{2((4n-6))}{3+4} + \frac{2(2n)}{3+6}$$

$$= \frac{1}{1890}(1589490 + 6717n)$$

$$(v) ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$$

$$= n\left(\frac{6\times 6}{6+6}\right) + 7\left(\frac{4\times 4}{4+4}\right) + (4n-6)\left(\frac{4\times 6}{4+6}\right) + 14\left(\frac{2\times 4}{2+4}\right) + (4n-6)\left(\frac{2\times 6}{2+6}\right) + (4n-6)\left(\frac{3\times 4}{3+4}\right) + 2n\left(\frac{3\times 6}{3+6}\right) = \frac{1}{105}(3093n - 107)$$

$$(vi) {}^{m}M_1(G) = \sum_{u \in V(G)} \frac{1}{d_G(u)^2}$$

$$= 2(n+2)\left(\frac{1}{2^2}\right) + 2(n+2)\left(\frac{1}{4^2}\right) + 2(n-1)\left(\frac{1}{3^2}\right) + 2(n-1)\left(\frac{1}{6^2}\right)$$

$$= \frac{1}{144}[90(n+2) + 40(n-1)]$$

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) d_G(v)}$$

$$= n\left(\frac{1}{6\times 6}\right) + 7\left(\frac{1}{4\times 4}\right) + (4n-6)\left(\frac{1}{4\times 6}\right) + 14\left(\frac{1}{2\times 4}\right) + (4n-6)\left(\frac{1}{2\times 6}\right) + (4n-6)\left(\frac{1}{4\times 3}\right) + 2n\left(\frac{1}{3\times 6}\right) = \frac{1}{576}[540 + 560n]$$

$$(vii) HM_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2$$

$$= n(6+6)^2 + 7(4+4)^2 + (4n-6)(4+6)^2 + 14(2+4)^2 + (4n-6)(2+6)^2 + (4n-6)(3+4)^2 + 2n(3+6)^2 = 1158n - 326$$

$$HM_2(G) = \sum_{uv \in E(G)} [d_G(u) d_G(v)]^2$$

$$= n(6\times 6)^2 + 7(4\times 4)^2 + (4n-6)(4\times 6)^2 + 14(2\times 4)^2 + (4n-6)(2\times 6)^2 + (4n-6)(3\times 4)^2 + 2n(3\times 6)^2 = 5400n - 2496$$

Example 3.2:

Consider the graph $G = S(L_5(\alpha, \beta))$. Then we have, $\left|V\left(S(L_5(\alpha,\beta))\right)\right| = 44; \left|E\left(S(L_5(\alpha,\beta))\right)\right| = 78$. Here $|V_2| = |V_4| = 14$ and $|V_3| = |V_6| = 8$. Also there are 5 edges with degrees of end vertices(6,6); 7 edges with degrees of end vertices(4,4);14 edges with degrees of end vertices(4,6); 14 edges with degrees of end vertices(2,4);14 edges with degrees of end vertices(2,6);14 edges with degrees of end vertices(3,4);10 edges with degrees of end vertices(3,6). Hence

$$(i) M_1(G) = 640$$

$$M_2(G) = 1136$$

$$(ii) R(G) = 2.830$$

$$(iii) X(G) = 8.775$$

$$(iv) H(G) = 19.772$$

$$(v) ISI(G) = 146.27$$

$$(vi) {}^{m}M_1(G) = 5.486$$

$${}^{m}M_2(G) = 5.7986$$

$$(vii) HM_1(G) = 5464$$

$$HM_2(G) = 22712$$

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