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Nullity of Expanded Smith graphs

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Abstract

A smith graph is a graph whose at least one eigenvalue is 2. There are 6 types of smith graph $C_n(n \geq 3), W_n(n \geq 6), S_5 = K_{1,4}, H_7, H_8 \text{ and } H_9$. In this paper we have discussed the nullity of expanded smith graphs ($W_n(n \geq 6), S_5 = K_{1,4}, H_7, H_8 \text{ and } H_9$). We have also evaluated the nullity of graph is applicable for the isomorphic molecules of unsaturated conjugate hydrocarbons.

keywords: smith graphs; nullity; sequential joins; expanded graphs.

1 Introduction

In mathematics and computer science, graph theory is the study of graphs, mathematical relationships between objects are used to model pairwise. A graph consists of nodes which are connected by arcs. Algebraic graph theory is the extension of the graph theory whose methods are applicable to many problems about graphs. There are three main branches of algebraic graph theory. The first branch of algebraic graph theory studies the spectrum of the adjacency or laplacian matrix of a graph. It is known as the spectral graph theory. Spectral graph theory is the study of properties of graphs in relationship to the characteristic polynomials, eigenvalues and eigenvectors of matrices associated with graphs. In a theory of graph spectra, some special types of graphs and their characteristics are studied in detail. The second branch of algebraic graph theory, especially with regard to automorphism groups and geometric group theory includes the study of graphs. The third branch of algebraic graph theory concerns algebraic properties of invariants of graphs.

Suppose G = (V, E) be a smith graph with vertex set V(G) and edge set E(G) each element of E identify with an unordered pair of elements of $V = \{v_1, v_2, \ldots, v_n\}$ whose at least one eigenvalue is 2. Smith graph has play an important role in spectral graph theory. There are 6 types of smith graphs as shown in below figure (1).

The adjacency matrix of a graph G with n vertices is

$$A(G) = \begin{cases} 1, & if\ v_i\ is\ adjacent\ to\ v_j \\ 0, & otherwise. \end{cases}$$

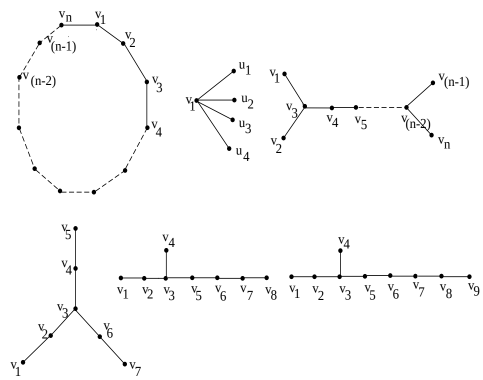

Figure 1: $C_n(n \geq 3), S_5 = K_{1,4}, W_n(n \geq 6), H_7, H_8 \ and \ H_9$

Nullity of graph $\eta(G)$ = |(G)|- r(A(G)), where r(A(G)) is the rank of adjacency matrix and |(G)|is the order of the graph i.e. number of vertices in G.
A non- trivial vertex weighting of a graph G is called a zero- sum weighting provided that for each vertex $v \in G, \Sigma f(u) = 0$, where the summation is taken over all $u \in N_G(v)$, and $N_G(v)$ is the neighbor vertex set of v.
Out of all zero- sum weightings of a graph G, a high zero- sum weighting of G is one that uses maximum number of non- zero independent variables. Nullity can also be defined as maximum number of independent variable in high zero sum weighting. Symbol of nullity η is firstly introduced by Ivan Gutman in 1970. Nullity is pertinent for the stability of unsaturated hydrocarbons with $\eta(G) > 0$ is anticipated to have an open shell electron configuration.
The sequential join of n disjoint graphs $G_1, G_2, \ldots, G_n$ is the graph $(G_1 + G_2)U(G_2 + G_3)U \ldots U(G_{n-1} + G_n)$ and denoted by$\sum_{i=1}^{n} G_i$, for i= 1,2,..., n, whose vertex and edge sets are defined as follows:

$$V(\sum_{i=1}^{n} G_i) = \bigcup_{i=1}^{n} V(G_i)$$

$$E(\sum_{i=1}^{n} G_i) = \{\bigcup_{i=1}^{n} E(G_i)\} \cup \{uv : \forall \ u \in G_i \ and \ v \in G_{i+1} : i = 1, 2, \ldots n-1\}$$

Then the sequential join of any graph is known as an expanded graph.
Nullity is very applicable for the stability of unsaturated conjugate hydrocarbons molecules by Huckel molecular orbital theory (HMO). According to HMO theory arises following two cases:

1. If $\eta(G) > 0$ then the isomorphic chemical molecule is more reactive, unstable.

2. If $\eta(G) = 0$ then the isomorphic chemical molecule is stable, less reactive.

Rest of the paper is organized as follows: In section 3, we have evaluated the nullity of expanded smith graphs $W_n(n \geq 6), H_7, H_8 \ and \ H_9, S_5 = K_{1,4}$. We have given the conclusions of all results in section 4.

2 Related Work

Spectral graph theory visioned during the two decades starting from 1940 to 1960. "The theory of graph spectra" written by Cvetkovic, D. M. et al. (1980), has included the monograph of the research area of spectral graph theory and further updated newer results in the theory of graph spectra (1989).In the preceding 9 -10 years, many developments in this arena such as Lubotzky, A. et al. (1988) gave isometric properties of expander graphs. Currently developed spectral techniques are more powerful and convenient for well- established graph.Gutman, I. (2001) has shown in his paper that nullity of the line graph of tree i.e. $\eta L(T)$ is at most one.Boravicanin, B. and Gutman, I. (2011) in their paper related to the nullity of graphs, explained the chemical importance of graph- spectrum based on Huckel molecular orbital theory and recently obtained general mathematical results on the nullity of graphs $\eta(G)$.Barrette, W. et al. (2014) have found the maximum nullity of a complete subdivision graph. Gu, R. et. al. (2014) have done the research on randic incidence energy of graphs. Sharaf, K. R. and Rasul, K. B. (2014) gave results on the nullity of expanded graphs and Sharaf, K. R. and Ali, D. A. (2014) have given nullity of t- tupple graphs.S. (2014) has shown the expression of the nullity set of unicyclic graphs is depend on the extremal nullity.

3 Nullity of expanded smith graphs

Theorem 3.1: Nullity of sequential join of smith graphs are

$$\eta(\sum_{i=1}^{m} W_p) = \begin{cases} 2m, & p = 2n+4, where\ m, n\ are\ positive\ integers\ and\ n \geq 1 \\ 3m, & p = 4n+1, where\ m, n\ are\ positive\ integers\ and\ n \geq 2 \\ 2m+1, & p = 4n-1, where\ m\ is\ odd\ integers\ and\ n \geq 2 \\ 2m, & p = 4n-1, where\ m\ is\ an\ even\ integers\ and\ n \geq 2 \end{cases}$$

Proof: Case (i): Consider a smith graph W_{2n+4}. Now let the m copies of $W_{(2n+4)}$ with vertex set $\{v_{11}, v_{12}, \ldots, v_{1(2n+4)}\}$, $\{v_{21}, v_{22}, \ldots, v_{2(2n+4)}\}$,..., $\{v_{m1}, v_{m2},\ldots, v_{m(2n+4)}\}$ and edge set $\{e_{11}, e_{12},\ldots, e_{1(2m+3)}\}$, $\{e_{21}, e_{22}, \ldots, e_{2(2n+3)}\}$, ..., $\{e_{m1}, e_{m2},\ldots, e_{m(2m+3)}\}$ respectively. Then the sequential join of these m copies can be shown in figure 1.

For finding the nullity of $\sum_{i=1}^{m} W_{2n+4}$, we apply co- neighbor lemma [5] on given graph. (v_{11}, v_{12}), ($v_{1(2n+3)}$, $v_{1(2n+4)}$),(v_{21}, v_{22}), ($v_{2(2n+3)}, v_{2(2n+4)}$),..., (v_{m1}, v_{m2}), ($v_{m(2n+3)}, v_{m(2n+4)}$) are pairs of co- neighbor vertices in $\sum_{i=1}^{m} W_{2n+4}$. Nullity of graph = nullity of remaining graph +

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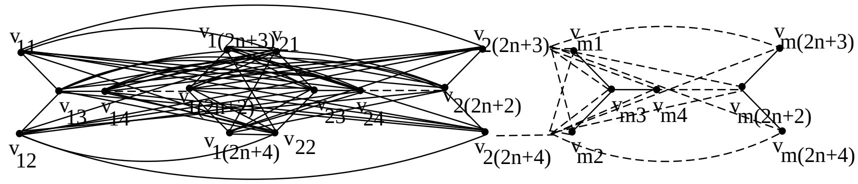

Figure 2: $\sum_{i=1}^{m}(W_{2n+4})$

number of removed vertices. Therefore, $\eta(\sum_{i=1}^{m} W_{2n+4}) = \eta(\sum_{i=1}^{m} P_{2n+2})$ + 2m = 0 +2m. Hence, $\eta(\sum_{i=1}^{m} W_{2n+4})$ = 2m, where m , n are positive integers and $n \geq 1$.

Case (ii): Consider a smith graph W_{4n+1}. Now we consider the m copies of W_{4n+1} with vertex set $\{v_{11},\ v_{12},\ldots,\ v_{1(4n+1)}\}$, $\{v_{21},\ v_{22},\ldots,\ v_{2(4n+1)}\},\ldots,\ \{v_{m1},\ v_{m2},\ldots,\ v_{m(4n+1)}\}$ and edge set $\{e_{11}, e_{12}, \ldots, e_{1(4n)}\}$, $\{e_{21},\ e_{22},\ldots,e_{2(4n)}\},\ldots,\ \{e_{m1},\ e_{m2},\ldots,\ e_{m(4n)}\}$ respectively. Sequential join of these m copies shown in figure 2.

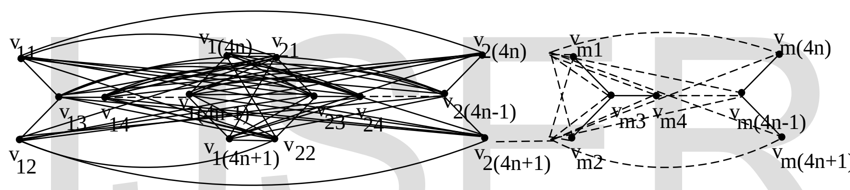

Figure 3: $\sum_{i=1}^{m}(W_{4n+1})$

For determing the nullity of graph, we apply co-neighbor lemma [5]. $(v_{11},\ v_{12})$, $(v_{1(2n+3)}, v_{1(4n+1)})$,$(v_{21},\ v_{22})$, $(v_{2(2n+3)},\ v_{2(4n+1)}),\ldots,$ (v_{m1},v_{m2}), $(v_{m(2n+3)},\ v_{m(4n+1)})$ are pairs of co-neighbor vertices. Nullity of graph = nullity of remaining graph + number of removed vertices. Therefore, $\eta(\sum_{i=1}^{m} W_{4n+1}) = \eta(\sum_{i=1}^{m} P_{4n-1})$ + 2m = 3m. Hence, $\eta(\sum_{i=1}^{m} W_{4n+1})$ = 3m, where m, n are positive integers and $n \geq 2$.

Case (iii): We consider two sub-cases as follows: case(a)if number of copies of smith graphs are odd and case (b)if number of copies of smith graphs are even.

case (a): If numbers of copies of smith graph are odd. Let the number of copies m be 2t-1 (odd). W_{4n-1} with vertex set $\{v_{11},\ v_{12},\ldots,\ v_{1(4n-1)}\}$, $\{v_{21},\ v_{22},\ldots,\ v_{2(4n-1)}\},\ldots,\ \{v_{(2t-1)1}, v_{(2t-1)2},\ldots,\ v_{(2t-1)(4n-1)}\}$ and edge set $\{e_{11},\ e_{12},\ldots,\ e_{1(4n-2)}\}$, $\{e_{21},\ e_{22},\ \ldots,e_{2(4n-2)}\},\ldots,$ $\{e_{(2t-1)1},\ e_{(2t-1)2},\ldots,\ e_{(2t-1)(4n-2)}\}$ respectively. Sequential join of these 2t -1 copies can be shown in below figure 3.

For, the nullity of $(\sum_{i=1}^{2t-1} W_{4n-1})$, we apply co-neighbor lemma [5]. Nullity of graph = nullity

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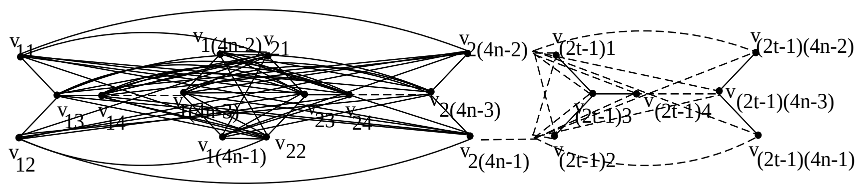

Figure 4: $\sum_{i=1}^{2t-1}(W_{4n-1})$

of remaining graph + number of removed vertices. Therefore, $\eta(\sum_{i=1}^{2t-1} W_{4n-1}) = \eta(\sum_{i=1}^{2t-1} P_{4n-3})$ + 2(2t-1) = 1 +4t-2 = 4t-1.

Hence $\eta(\sum_{i=1}^{m} W_{4n-1}) = 2m + 1$, where m is an odd positive integer.

case (b): If numbers of copies of smith graph are even. Let the number of copies m be 2t (even). Now we consider the 2t copies of $W_{(4n-1)}$ with vertices $\{v_{11},\ v_{12},\ldots,\ v_{1(4n-1)}\}$, $\{v_{21},\ v_{22},\ldots,\ v_{2(4n-1)}\}$,..., $\{v_{(2t)1},\ v_{(2t)2},\ \ldots,\ v_{2t(4n-1)}\}$ and edges $\{e_{11},\ e_{12},\ \ldots,\ e_{1(4n-2)}\}$, $\{e_{21},\ e_{22},\ldots,e_{2(4n-2)}\}$,..., $\{e_{(2t)1},\ e_{(2t)2},\ \ldots,\ e_{2t(4n-2)}\}$ respectively. Sequential join of these 2t copies shown in figure.

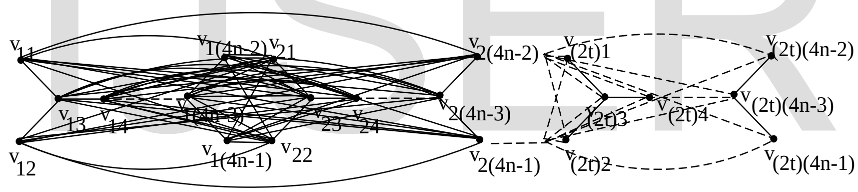

Figure 5: $\sum_{i=1}^{2t}(W_{4n-1})$

For finding the $\eta(\sum_{i=1}^{2t} W_{4n-1})$, we apply co- neighbor lemma [5] in the graph $(\sum_{i=1}^{2t} W_{4n-1})$ (v_{11}, v_{12}), $(v_{1(4n-2)},\ v_{1(4n-1)})$,$(v_{21},\ v_{22})$, $(v_{2(4n-2)},\ v_{2(4n-1)})$,..., $(v_{(2t)1},\ v_{(2t)2})$, $(v_{2t(4n-2)},\ v_{2t(4n-1)})$ are the pairs of co- neighbor vertices. Nullity of graph = nullity of remaining graph + number of removed vertices. Therefore, $\eta(\sum_{i=1}^{2t} W_{4n-1}) = \eta(\sum_{i=1}^{2t} P_{4n-3})$ + 2(2t) = 0 +4t = 4t.

Hence $\eta(\sum_{i=1}^{m} W_{4n-1})$= 2m, where m is an even positive integer.

Theorem 3.2: Nullity of sequential join of smith graph H_7 as follows:
Case (i): If numbers of copies are odd i.e. 2m+1

$$\eta(\sum_{i=1}^{2m+1} H_7) = 2.$$

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Case (ii): If numbers of copies are even i.e. 2m

$$\eta(\sum_{i=1}^{2m} H_7) = 1.$$

Proof: Case(i): Consider a smith graph H_7 with vertex set V= $\{v_1, v_2, ..., v_7\}$ and edge set E= $\{e_1, e_2, ..., e_6\}$respectively. We apply sequential join on (2m+1) copies of smith graph H_7 with $v_{11}, v_{12}, ..., v_{17}, v_{21}, v_{22}, ..., v_{27}, ..., v_{(2m+1)1}, v_{(2m+1)2}, ..., v_{(2m+1)7}$ and $e_{11}, e_{12}, ..., e_{16}, e'_{11}, e'_{12}, ...\ e_{17}, ..., e_{(2m+1)1}, e_{(2m+1)2}, ..., e_{(2m+1)6}$ vertices and edges respectively.

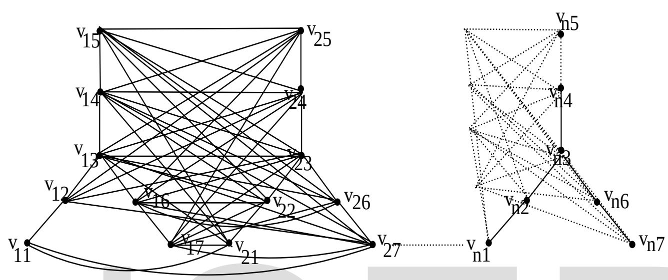

Figure 6: $\sum_{i=1}^{2m+1} (H_7)$

Now we determining the nullity of $\sum_{i=1}^{2m+1} H_7$. The nullity $\eta(G) = |$(G)$|$- r(A(G)) The *adjacency matrix* $A[(\sum_{i=1}^{2m+1} H_7)]$ of the $7(2m+1) \times 7(2m+1)$ order

$$A(\sum_{i=1}^{2m+1} H_7) = \begin{bmatrix} A & B & O & \dots & \dots & O & O \\ B & A & B & \dots & \dots & O & O \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ O & O & O & \dots & \dots & A & B \\ O & O & O & \dots & \dots & B & A \end{bmatrix}$$

Where, A, B, O is the 7×7 order matrix

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

$$O = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

If numbers of copies are odd then $\eta(\sum_{i=1}^{2m+1} H_7)$ = 7(2m+1) - (14m+ 5) = 2. **Case (ii):** If numbers of copies are even i.e. 2m. Similarly as above case(i) then $\eta(\sum_{i=1}^{2m} H_7)$ = 7(2m) - (14m-1) = 1.

Theorem 3.3: Nullity of sequential join of H_8 is n i.e. $\eta(\sum_{i=1}^{n} H_8) = n$.

Proof: Consider a smith graph H_8 with vertex set V= $\{v_1, v_2, ..., v_8\}$ and edge set E= $\{e_1, e_2..., e_7\}$ respectively. We apply sequential join on n copies of smith graph H_8 with $v_{11}, v_{12}, ..., v_{18}, v_{21}, v_{22}, ..., v_{28}, ..., v_{n1}, v_{n2}, ..., v_{n8}$ and e_{11}, e_{12},..., e_{17}, e'_{11}, e_{12},... e_{18},...,$e_{(n-1)1}$, $e'_{(n-1)2}$,...,$e_{(n-1)8}$, e_{n1}, e_{n2}, ...,e_{n7} vertice and edges respectively. Now we finding the nullity of sequential join of smith graph H_8 is the number of non zero independent variables in any of its high zero- sum weightings. Firstly we consider one copy of H_8. The weighting for the H_8 is a high zero sum weighting that uses only one independent non - zero variable, hence $\eta(H_8)$ = 1. Now we consider the two copies of H_8 with sequential joins then we use 2 independent non - zero variables, hence $\eta(H_8 + H_8) = 2$. We continue this process for n copies of H_8 with sequential joins. We use n independent non - zero variables, hence $\eta(\sum_{i=1}^{n} H_8) = n$.

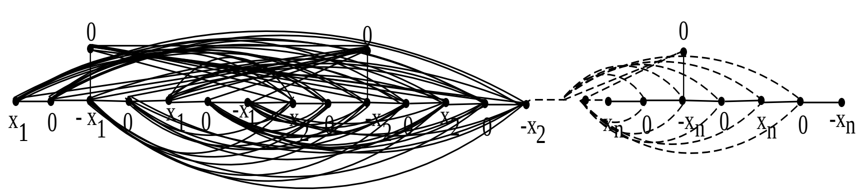

Figure 7: $\sum_{i=1}^{m}(H_8)$

Theorem 3.4: Nullity of sequential join of H_9 is n i.e.$\eta(\sum_{i=1}^{n} H_9) = n$.

Proof: Consider a smith graph $H_9$with vertex set V= $\{v_1, v_2, \ldots, v_9\}$ and edge set E= $\{e_1, e_2 \ldots, e_8\}$ respectively. We apply sequential join on n copies of smith graph $H_9$with $v_{11}, v_{12}, ..., v_{19}, v_{21}, v_{22}, ..., v_{29}, ..., v_{n1}, v_{n2}, ..., v_{n9}$ and e_{11}, e_{12},..., e_{18}, $e^{'}_{11}$, $e^{'}_{12}$,... e_{19},...,$e^{'}_{(n-1)1}$, $e^{'}_{(n-1)2}$,... $e^{'}_{(n-1)9}$, e_{n1}, e_{n2},...,e_{n8} vertices and edges respectively.

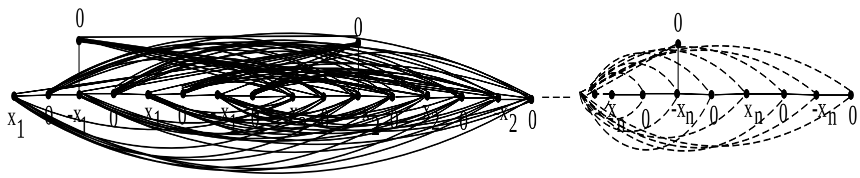

Figure 8: $\sum_{i=1}^{m}(H_9)$

Now we determining the nullity of sequential join of smith graph H_9 is the number of non zero independent variables in any of its high zero- sum weightings. Firstly we consider one copy of H_9. The weighting for the H_9 is a high zero sum weighting. We use only one independent non zero variable, hence $\eta(H_9) = 1$. Now we consider the two copies of H_9 with sequential joins then we use 2 independent non- zero variables, hence $\eta(H_9 + H_9) = 2$. We continue this process for n copies of H_9 with sequential joins. We use n independent non-zero variables, hence $\eta(\sum_{i=1}^{n} H_9) = n$.

Theorem 3.5: Nullity of sequential join of $K_{1,4}$ is 3n i.e. $\eta(\sum_{i=1}^{n} K_{1,4}) = 3n$

Proof: Consider a smith graph $K_{1,4}$ with vertex set V= $\{v_1,\ u_1,\ u_2,\ u_3,\ u_4\}$ and edge set E= $\{e_1,\ e_2,\ e_3,\ e_4\}$ respectively.

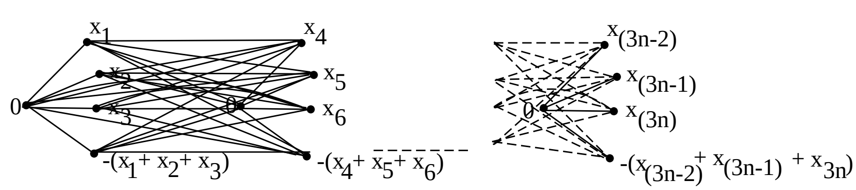

Figure 9: $\sum_{i=1}^{m}(K_{1,4})$

We apply sequential join on n copies of smith graph $K_{1,4}$with v_{11}, v_{12}, ..., v_{15}, v_{21}, v_{22},..., v_{25}, ..., v_{n1}, v_{n2}, ..., v_{n5} and e_{11}, e_{12}, ..., e_{14}, $e^{'}_{11}$, $e^{'}_{12}$, ... $e^{'}_{15}$,...,$e^{'}_{(n-1)1}$, $e^{'}_{(n-1)2}$,..., $e^{'}_{(n-1)5}$, e_{n1}, e_{n2}, ...,e_{n4} vertices and edges respectively.

Now we finding the nullity of sequential join of smith graph $K_{1,4}$ is the number of non - zero independent variables in any of its high zero sum weightings. Firstly we consider one copy of $K_{1,4}$. The weighting for the $K_{1,4}$ is a high zero sum weighting that uses only three independent non zero variable, hence $\eta(K_{1,4}) = 3$. Now we consider the two copies of $K_{1,4}$ with sequential joins then we use 6 independent non- zero variables, hence $\eta(K_{1,4} + K_{1,4}) = 3+3$. We continue this process for n copies of $K_{1,4}$ with sequential joins. We use 3n independent non- zero variables, hence $\eta(\sum_{i=1}^{n} K_{1,4}) = 3n$.

4 Conclusions

We have evaluated the nullity for expanded smith graphs $\eta(G)$ which is greater than 0. If $\eta(G) > 0$ then the respective molecule is an unstable, open shell and highly reactive. Therefore, we have conclude that if any chemical compound, whose structure is isomorphic to expanded smith graphs then it will be unstable, highly reactive and it will have open shell electron configuration.

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