Nullity and Energy Bounds of Central Graph of Smith Graphs

Usha Sharma[1], Renu Naresh[2]

[1, 2] Department of Mathematics and Statistics, Banasthali University, Banasthali Rajasthan, India

Abstract: ***A smith graph G is a graph whose at least one eigenvalue is 2. The η nullity (G) of a graph G is the multiplicity of the eigenvalue 0 in the spectrum of adjacency matrix of graph A (G). Energy of the graph is the sum of the absolute values of the Eigen values of the adjacency matrix G. Central graph C (G) of graph G is obtained by the subdividing each edge exactly once and joining all the non adjacent vertices of graph G. We have evaluated the nullity and the energy bounds of the central graph of smith graphs. By Huckel molecular Orbital theory, these spectral properties are applicable for determining the stability of unsaturated conjugate hydrocarbons which are isomorphic to central graph of smith graphs.***

Keywords: Smith graph, Central graph, Nullity, Energy, Huckel molecular Orbital theory

1. Introduction

Spectral graph theory is the study of properties of graphs in relationship to the characteristic polynomials, Eigen values and eigenvectors of matrices associated with graphs. In a theory of graph spectra, some special types of graphs are studied in detail and their characteristics are well known and summarized in [CvDSa]. Here we discussed the smith graphs. Smith graphs are C_n ($n \geq 3$), W_n ($n \geq 6$), $S_5 = K_{1,4}$, H_7, H_8 and H_9.

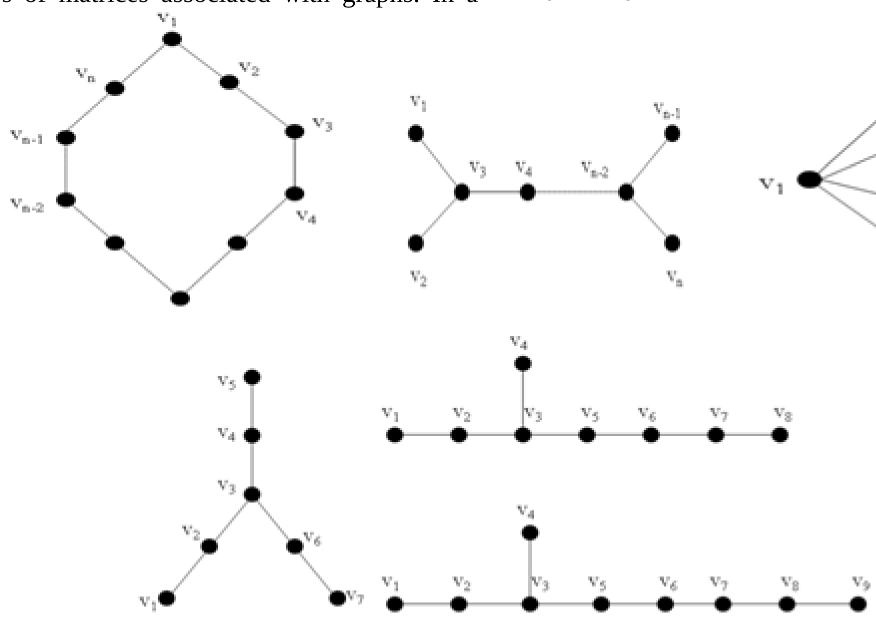

Figure 1: C_n; $n \geq 3$, W_n; $n \geq 6$, $S_5 = K_{1,4}$, H_7, H_8, H_9

The central graph C (G) of a graph G is obtained by subdividing each edge of G exactly once and joining all the nonadjacent vertices of G.

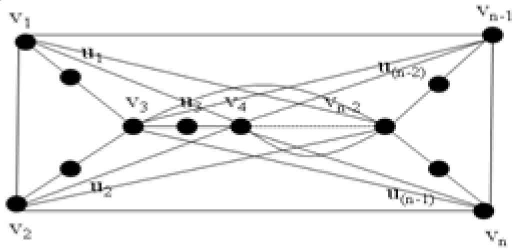

Figure 2: C (W_n)

Here, we have evaluated the nullity of a special type of graphs and also elaborated energy bounds. Let G be a graph of order n, having vertex set V (G) and edge set E (G). Let A (G) be the adjacency matrix of G, where

$$A(G) = \begin{cases} 1, & if\ v_i\ is\ adjacent\ to\ v_j \\ 0, & if\ v_i\ is\ not\ adjacent\ to\ v_j \end{cases}.$$

$$A[C(G)] = \begin{bmatrix} 0 & 1 & 1 & 0 & \cdots & \cdots & 1 \\ 1 & 0 & 0 & 0 & \cdots & \cdots & 1 \\ 1 & 0 & 0 & 1 & \cdots & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & \cdots & 1 \\ 1 & 1 & 1 & 1 & \cdots & \cdots & 1 \end{bmatrix}_{(n\times n)}$$

A scalar λ is called an eigenvalue of the square matrix A (G) if there exist a nonzero vector X such that AX = λX, where X is called an eigenvector corresponding to the eigenvalue λ. In other words, Eigen values are the set of scalars which is associated with a characteristic equation of adjacency matrix of graph G that is $|A- \lambda I| = 0$, where I is the identity matrix.

Nullity of G is the zero multiplicity of an eigenvalue in the spectrum of A(G). It is firstly introduced by Gutman in his paper.
The chemical importance of this graph spectrum based invariant lies in the fact, that within the Huckel molecular orbital model, if η(G) > 0 for the molecular graph G, then the corresponding chemical compound is highly reactive and unstable or nonexistent and if η(G) = 0 then the respective molecule is predicted to have a stable, closed-shell, electron configuration and low chemical reactivity.

In 1940's energy introduced by chemistry. Ivan Gutman, (1978) interpreted the energy of graph in first time. However, the inspirations for his definition vision much earlier, in the 1930's, when Erich Huckel recommended the famous Huckel Molecular Orbital Theory. Huckel's method permits chemists to approximate energies related with π-electron orbital's in a special group of molecules called conjugated hydrocarbons. The method assumes that the Hamiltonian operator is a simple linear combination of certain orbital, and given the time-independent Schrodinger equation to solve for the energies desired (2012).

Gunthard, H. H. and Primas, H. (1956) realized that the matrix is applicable in the Huckel method is a first degree polynomial of the adjacency matrix of a certain graph related to the molecule being studied.

Moreover, under certainly reasonable speculation about the molecule, its total π-electron energy can be written as the energy of the graph is the sum of the absolute values of the Eigen values λ of the adjacency matrix A(G) that is E(G) = $\sum_{i=1}^{n}|\lambda_i|$ is related to the total π-electron energy in a molecular graph.

We have appraised the energy bounds of the graph with the help of Schwartz inequality. Let $a_1,\ldots, a_n$ and $b_1,\ldots, b_n$ be the two sequences. Then

$$\left|\sum_{i=1}^{n} a_i b_j\right|^2 \le \left(\sum_{i=1}^{n}|a_i|^2\right)\left(\sum_{i=1}^{n}|b_i|^2\right)$$

Rest of the paper in section 2 we have given related work to nullity and energy of graphs. We use one proposition in this paper. we have mentioned in section 3. In section 4, we have determined new results on the nullity of the central graph of smith graphs. In section 5, we have evaluated energy bounds of central graph of smith graph. We have concluded the results in section 6.

2. Literature Review

Spectral graph theory vision 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 the tree that is ηL(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 η(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.

Coulson, C. A. and et al. (1978) explained some graphical aspects of Huckel theory and also explained the energy level of the graph. Biggs, N. (1993) discussed the applications of linear algebra and matrix theory in Algebraic graph theory. Gutman, I. (2001) presented fundamental mathematical results on E and relation between E(G) and characteristic polynomial of G and bounds for E. Bo, Z.(2004) presented upper bound for the energy of a graph in terms of a degree sequence and specified maximal energy graph and maximal energy bipartite graph. Adiga, C. and et al. (2007) determined the several classes of graphs such as biregular, molecular graphs, triregular graphs satisfy the condition E(G) > n. Gutman, I. and et al. (2012) explicated the chemical origin of the graph energy concept and briefly survey of applications of total π-electron energy. Gutman, I. and et al. (2015) shown that for a fixed value of n, both the spectral radius and the energy of complete p- partite graphs are minimal for complete split graph CS(n, p-1) and are maximal for Turan graph T(n, p). Song Y. Z. and et al. (2015) proved that the nullity of the bipartite graph that is η(G) = |G|-2- 2 $In_2(\Delta(G))$, if G is a reduced bipartite graph.

3. Preposition

Proposition 3.1: Let G be a graph and $\lambda_1, \lambda_2,\ldots \lambda_n$ are the Eigen values of adjacency matrix A(G), then $\sum_{i=1}^{n}\lambda_i^2 = 2.\textit{number of edges}$

4. Nullity of Central graph of Smith graphs

We will discuss the nullity of central Graph of different types of smith graph out of these many are nonsingular.

Theorem 4.1: Nullity of central graph of smith graph W_n; $n \geq 6$ is zero, that is $\eta\ [C(W_n)] = 0\ \ \forall\ \ n \geq 6$.

Proof: Consider a smith graph W_n with vertex set V= $\{v_1, v_2, v_3, \ldots, v_n\}$ and edge set E= $\{e_1, e_2, e_3, \ldots, e_{(n-1)}\}$respectively. Then, $C(W_n)$ has vertex set $\{v_1, u_1, v_2, u_2, \ldots, v_{(n-2)}, u_{(n-1)}, v_{(n-1)}, u_{(n-1)}, v_n\}$ and edge set $\{e_1, e'_1, e_2, e'_2, \ldots, e_{(n-1)}, e'_{(n-1)}, \ldots, e_{12}, e_{14}, \ldots, e_{1(n-1)}, e_{24}, e_{25}, \ldots, e_{(2n-1)}, \ldots, e_{(n-1)(n-2)}\}$.

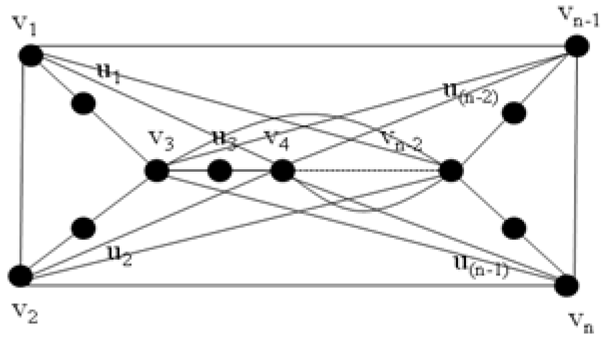

Figure 3: $C(W_n)$

Now the total number of vertices p in $C(W_n)$ = number of vertices in (W_n) + number of edges in (W_n)= n + (n-1) = 2n-1. The total number of edges q in $C(W_n)$ = 2(number of edges in W_n) + number of edges between non - adjacent vertices in W_n = 2(n-1) + number of edges in K_n - number of edges in $C(W_n)$ = 2(n-1) + $\frac{n(n-1)}{2}$ - (n-1) = $\frac{(n-1)(n+2)}{2}$. Now we find the nullity of graph $C(W_n)$.

Firstly we construct adjacency matrix

$$[a_{ij}]_{(2n-1)(2n-1)} = \begin{cases} 1, \text{ if } v_i \text{ is adjacent to } v_j \\ 0, \text{ if } v_i \text{ is not adjacent to } v_j \end{cases}$$

$$A[C(W_n)] = \begin{bmatrix} 0 & 1 & 1 & 0 & \cdots & \cdots & 1 \\ 1 & 0 & 0 & 0 & \cdots & \cdots & 1 \\ 1 & 0 & 0 & 1 & \cdots & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & \cdots & 1 \\ 1 & 1 & 1 & 1 & \cdots & \cdots & 1 \end{bmatrix}_{(2n-1)(2n-1)}$$

Now we apply elementary row operation for finding the nullity of the graph. Nullity of graph = |(G)| - r(A(G)), where r(A(G)) is the rank of matrix. Then, r(A(G)) = number of non – zero rows in the row reduced form of matrix = (2n-1). Then the nullity of graph = $|C(W_n)|$ - r(A(G)) = (2n-1) - (2n-1) = 0.

Therefore, $\eta\ [C\ (W_n)] = 0\ \ \forall\ \ n \geq 6$.

Theorem 4.2: Nullity of central graph of smith graph H_7 is zero, that is $\eta\ [C\ (H_7)] = 0$.

Proof: Consider a smith graph H_7 with vertex set V= $\{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and edge set E= $\{e_1, e_2, e_3, e_4, e_5, e_6\}$ respectively. Then, $C(H_7)$ has vertex set $\{v_1, u_1, v_2, u_2, \ldots, v_5, u_5, v_6, u_6, v_7\}$ and edge set $\{e_1, e'_1, e_2, e'_2, \ldots, e_6, e'_6, \ldots, e_{13}, e_{14}, \ldots, e_{17}, e_{24}, e_{25}, \ldots, e_{27}, \ldots, e_{56}, e_{57}\}$.

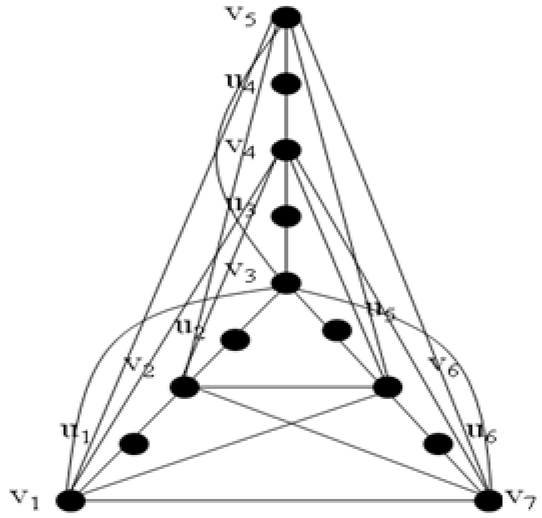

Figure 4: C (H_7)

Number of vertices in H_7 + number of edges in H_7 = 13 and the total number of edges in C (H_7) = 2(number of edges in H_7) + number of edges between non - adjacent vertices in H_7 = 12 + number of edges in K_7 - number of edges in H_7 = 12 + $\frac{7(7-1)}{2}$ - 6 = 27. Now we find the nullity of graph $C(H_7)$. Then, we construct the adjacency matrix A= $[a_{ij}]_{n \times n}$. The $A[C(H_7)]$ of the 13 × 13 order

$$\begin{bmatrix} 0&1&0&0&1&0&1&0&1&0&1&0&1 \\ 1&0&1&1&0&0&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&1&0&1&0&1&1&0 \\ 0&0&1&1&1&0&0&0&0&0&0&0&0 \\ 1&0&0&0&0&1&0&0&1&0&1&0&1 \\ 0&0&0&0&1&0&1&0&0&0&0&0&0 \\ 1&0&1&0&0&1&0&1&0&0&1&0&1 \\ 0&0&0&0&0&0&1&0&1&0&0&0&0 \\ 1&0&1&0&1&0&0&1&0&0&1&0&1 \\ 0&0&0&0&1&0&0&0&0&0&1&0&0 \\ 1&0&1&0&1&0&1&0&1&1&0&1&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&1 \\ 1&0&1&0&1&0&1&0&1&0&0&1&0 \end{bmatrix}_{13 \times 13}$$

We apply elementary row operation for determined the nullity of graph. Nullity of graph = |(G)| - r(A(G)), where r(A(G)) is the rank of matrix. The rank of graph = number of non – zero row in the row reduced form of matrix = 13. Therefore, $\eta\ [C\ (H7)] = 0$.

Theorem 4.3: Nullity of central graph of smith graph H_8 is zero. i.e. $\eta\ [C\ (H_8)] = 0$.

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. Then, C (H_8) has vertex set {v_1, u_1, v_2, u_2,…, u_7, v_8} and edge set {e_1, e'_1, e_2, e'_2,…, e_7, e'_7, e_{13}, e_{14},…, e_{18}, e_{24}, e_{25},…, e_{28},…, e_{68}}.

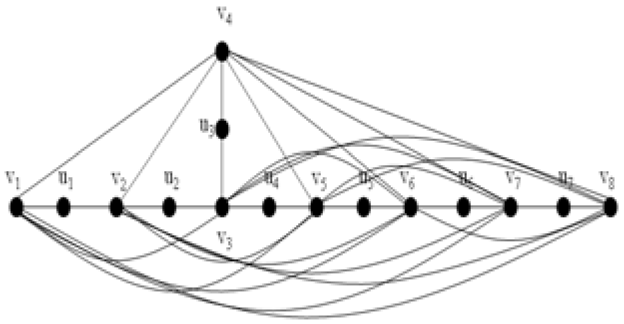

Figure 5: C (H_8)

Now the total number of vertices in C (H_8) = number of vertices in H_8 + number of edges in H_8 = 15 and the total number of edges in C (H_8) = 2(number of edges in H_8) + number of edges between non - adjacent vertices in H_8 = 14 + number of edges in K_8 - number of edges in H_8 = 14 + $\frac{8(8-1)}{2}$ - 7 = 35. Now we find the nullity of graph C (H_8). Firstly we construct the adjacency matrix A = $[a_{ij}]_{15\times15}$. We apply elementary row operation for rank. Nullity of graph = |(G)|- r(A(G)), where r(A(G)) is the rank of matrix. Then, the rank of matrix = number of non – zero row in the row reduced form of matrix = 15. Therefore, η [C (H_8)] = 0.

Theorem 4.4: Nullity of central graph of smith graph S_5 is zero. i.e. η [C (S_5)] = 0.

Proof: Consider a smith graph S_5 with vertex set V_1= v_1 and V_2= {u_1, u_2, u_3, u_4} and edge set E= {e_1, e_2, e_3, e_4} respectively. Then, C(S_5) vertex set {v_1, w_1, u_1, w_2, u_2, w_3, u_3,w_4, u_4} and edge set {e_1, e'_1, e_2, e'_2 , e_3, e'_3, e_4, e'_4, e_{12}, e_{13}, e_{14}, e_{23}, e_{24}, e_{34}}.

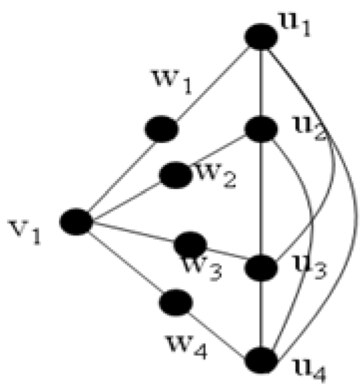

Figure 6: C(S_5)

Now the total number of vertices in C(S_5) = number of vertices in S_5 + number of edges in S_5 = 9 and the total number of edges in C(S_5) = 2(number of edges in S_5) + number of edges between non - adjacent vertices in S_5 = 8 + number of edges in K_5 – number of edges in S_5 = 8 + $\frac{5(5-1)}{2}$ - 4= 14. Now we find the nullity of graph C($K_{1,4}$). Firstly we construct the adjacency matrix A= $[a_{ij}]_{9\times9}$. We apply elementary row operation for rank. Nullity of graph = |(G)|- r(A(G)), where r(A(G)) is the rank of matrix. Then, the rank of matrix = number of non – zero row in the row reduced form of matrix = 9. Therefore, η [C(S_5)] = 0.

Theorem 4.5: Nullity of central graph of smith graphs H_9 is one. i.e. η [C(H_9)] = 1.

Proof: Consider a smith graph H_9 with vertex set V= {v_1, v_2,…, v_9} and edge set E= {e_1, e_2,…, e_8} respectively. Then, C(H_9) has vertex set {v_1, u_1, v_2, u_2,…, u_8, v_9} and edge set {e_1, e'_1, e_2, e'_2,…, e_7, e'_7, e_{13}, e_{14},…, e_{19}, e_{24}, e_{25},…, e_{29},…, e_{79}}.

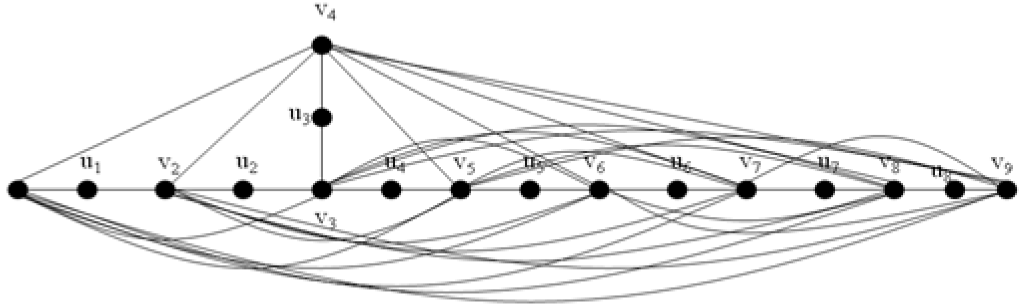

Figure 7: C(H_9)

Now the total number of vertices in C(H_9) = number of vertices in H_9 + number of edges in H_9 = 17 and the total number of edges in C(H_9) = 2(number of edges in H_9) + number of edges between non - adjacent vertices in H_9 = 16 + number of edges in K_9 - number of edges in H_9 = 16 + $\frac{9(9-1)}{2}$ - 8 = 44. Now we find the nullity of graph C(H_9). Firstly we construct the adjacency matrix A= $[a_{ij}]_{17\times17}$. We apply elementary row operation for rank. Nullity of graph = |(G)|- r(A(G)), where r(A(G)) is the rank of matrix. Then, the rank of matrix = number of non – zero row in the row reduced form of matrix = 16. Therefore, η [C(H_9)] = 1.

Theorem 4.6: Nullity of central graph of smith graph C_n ; n ≥ 3 are as follows:

$$\eta[C(C_n)] = \begin{cases} 0, if\ n\ is\ an\ odd\ positive\ int eger \\ 1, if\ n\ is\ an\ even\ positive\ int eger \end{cases}.$$

Proof: Consider a smith graph C_n with vertex set V= {v_1, v_2, v_3…, v_n} and edge set E= {e_1, e_2, e_3…, e_n} respectively. Then, C(C_n) vertex set {v_1, u_1, v_2, u_2,…, v_{n-2}, u_{n-1}, v_{n-1}, u_{n-1}, v_n}and edge set {e_1, e'_1, e_2, e'_2,…, e_n, e'_n,…, e_{12}, e_{14},…, $e_{1(n-1)}$, e_{24}, e_{25},…, $e_{2(n-1)}$,…, $e_{(n-2)\,n}$}.

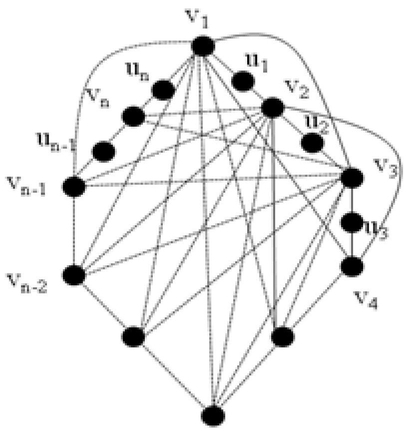

Figure 8: C(C_n)

Now the total number of vertices in C (C_n) = number of vertices in C_n + number of edges in C_n = 2n and the total number of edges in C (C_n) = 2(number of edges in C_n) + number of edges between non - adjacent vertices in C_n = 2n + number of edges in K_n - number of edges in C_n = 2n+ $\frac{n(n-1)}{2}$ - n = $\frac{n(n+1)}{2}$. Now we find the nullity of graph C(C_n). Firstly we construct the adjacency matrix A= $[a_{ij}]_{(n\times n)}$ of C_n, where n is an odd positive integer. Then the nullity of C (C_n) = |C (C_n)| - Rank of matrix =0 and if take n is an even number of vertices then the nullity of |C(C_n)| = |C(C_n)| - Rank of matrix =1.

5. Energy bounds of C (W_n); n ≥ 6, C (H_n); 7 ≤ n ≤ 9 and C (S_5)

Theorem 5.1: Let C (W_n) ∀ n ≥ 6, C (H_7), C (H_8), C (H_9), C (S_5) be the central graph of smith graphs. We denote these graphs by G. Then the energy bound of E (G) is

$$\sqrt{\left[(n-1)(n+2)+2(2n-1)(n-1)\left|\det A(C(G))\right|^{2/(2n-1)}\right]} \le E[C(G)] \le \sqrt{[(2n-1)(n-1)(n+2)]}$$

.

Proof: Upper Bound: Energy of given graph

$$E[C(G)] = \sum_{i=1}^{2n-1} |(\lambda_i)|$$

$$E^2[C(G)] = \left(\sum_{i=1}^{2n-1} |(\lambda_i)|\right)^2$$

$$E^2[C(G)] = \left(1.|\lambda_1| + 1.|\lambda_2| + 1.|\lambda_3| + \ldots + 1.|\lambda_{2n-1}|\right)^2$$

We use the Cauchy- Schwartz inequality to (1, 1, …, 1) and $(|\lambda_1|, |\lambda_2|, |\lambda_3|, \ldots, |\lambda_{2n-1}|)$ to get

$$\left(1.|\lambda_1| + 1.|\lambda_2| + \ldots 1.|\lambda_{2n-1}|\right)^2 = \left(|\lambda_1|^2 + |\lambda_2|^2 + \ldots\ |\lambda_{2n-1}|^2\right).(1+1+\ldots+1)$$

$$E^2[C(G)] \le \left(|\lambda_1|^2 + |\lambda_2|^2 + \ldots\ |\lambda_{2n-1}|^2\right).(1+1+\ldots+1)$$

$$E^2[C(G)] \le \sqrt{(2n-1)}\sqrt{\left(\sum_{i=1}^{2n-1} |\lambda_i|\right)^2}$$

$$E[C(G)] \le \sqrt{(2n-1)}\sqrt{[(n-1)(n+2)]} = \sqrt{[(2n-1)(n-1)(n+2)]} \qquad \ldots\ldots\ldots \quad (1)$$

Lower Bound: We use the arithmetic- geometric inequality

$$E[C(G)] = \sum_{i=1}^{2n-1} |\lambda_i|$$

$$E^2[C(G)] = \left(\sum_{i=1}^{2n-1} |\lambda_i|\right)^2$$

$$E^2[C(G)] = \sum_{i=1}^{2n-1} (|\lambda_i|)^2 + 2\sum_{i<j} |\lambda_i \lambda_j|$$

$$E^2[C(G)] \ge (n-1)(n+2) + (2n-1)(2n-2)\,A.M\left(|\lambda_i \lambda_j|\right)$$

$$E^2[C(G)] \ge (n-1)(n+2) + (2n-1)(2n-2)\,G.M\left(|\lambda_i \lambda_j|\right) \qquad \ldots \quad (2)$$

$$G.M\left(|\lambda_i \lambda_j|\right) = \left(\prod_{i<j} |\lambda_i \lambda_j|\right)^{2/(2n-1)(2n-2)}$$

$$G.M\left(|\lambda_i \lambda_j|\right) = \left(\prod_{i<j} |\lambda_i|^{(2n-1)}\right)^{2/(2n-1)(2n-2)}$$

$$G.M\left(|\lambda_i \lambda_j|\right) = \left(\prod_{i<j} |\lambda_i|\right)^{2/(2n-1)}$$

Put the values of G. M. in equation (2) then we have

$$E^2[C(G)] \geq (n-1)(n+2) + 2(2n-1)(n-1)\left|\det A[C(G)]\right|^{2/(2n-1)}$$

Therefore,

$$E[C(G)] \geq \sqrt{\left[(n-1)(n+2) + 2(2n-1)(n-1)\left|\det A(C(G))\right|^{2/(2n-1)}\right]} \quad \cdots\cdots\cdots \quad (3)$$

Now, from equation (1) and (4) then we get

$$\sqrt{\left[(n-1)(n+2) + 2(2n-1)(n-1)\left|\det A(C(G))\right|^{2/(2n-1)}\right]} \leq E[C(G)] \leq \sqrt{[(2n-1)(n-1)(n+2)]}.$$

6. Conclusions

We have interpreted that any chemical compound is isomorphic to the central graph of smith graphs except central graph of smith graph H_9 and C_n where n is an even are stable, closed – shell electron configuration and have low chemical reactivity and if any chemical compound is isomorphic to $C(H_9)$ and $C(C_n)$ are unstable, open shell electron configuration and the respective compound is highly reactive.

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