



## On the Spectral Parameters of certain Interconnection Networks, Nanosheets and Benzenoid Systems

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### ABSTRACT

Analysing graphs through the matrices associated to them have always yielded great outcomes. Modeling of chemical molecules as graphs enables us to predict their properties in an economically feasible way. Interpreting the spectral parameters of some known interconnection networks provides us a way to explore its graphical properties. This article attempts to find the spectral parameters of some variants of hypercube, nanosheets and benzenoid systems. Certain analytic expressions for these parameters have been derived in terms of their dimensions.

**Key words:** Variants of hypercube, chemical graphs, Nanosheets, Benzenoid systems, adjacency matrix, energy

### INTRODUCTION

Interconnection Networks are extremely important in designing computer networks that can be designed with minimum transmission delay, maximum fault tolerance, enhanced embeddability and more beneficial features. The spectral properties that are derived can be used to analyse various properties of these networks and can be exploited in various branches of computer science<sup>10</sup>.

Chemical graphs play a significant role in predicting the mathematical tools that correlate a molecule's chemical structure with its observed biological activity and physico-chemical property in a cost-effective manner<sup>6</sup>. To this end, certain spectral parameters of some variants of hypercube, benzenoid systems and nanosheets have been computed. It is observed that there exists a linear relationship between the dimensions of the graphs and their energy. Further, the results in this article



substantiate the fact all the molecular graphs whose degree of the vertices do not exceed three, are all non-hyperenergetic. Thus, this article explains how the behaviour of adjacency matrices creates an impact in the chemical properties of a molecule.

### Preliminaries

This section deals with all the prerequisites that are essential for the understanding of this article.

#### Definition 1<sup>5</sup>

The sum of the absolute values of the eigenvalues of the adjacency matrix of a graph  $G$  is termed as the energy,  $E(G)$  of a graph  $G$ .

#### Definition 2<sup>4,12</sup>

The largest and the smallest eigenvalues from the adjacency matrix of a graph  $G$  are referred to as the *spectral radius* or *index* and the least eigenvalue of  $G$  respectively<sup>4,12</sup>.

#### Definition 3<sup>7</sup>

The difference between the spectral radius and the least eigenvalue of  $G$  is called the *spread* of  $G$  and the difference between the spectral radius and the second largest eigenvalue is termed as *separator* of  $G$ <sup>7</sup>.

#### Definition 4<sup>8</sup>

A hyperenergetic graph is one whose energy is greater than twice one less than the number of vertices<sup>8</sup>.

#### Definition 5<sup>1</sup>

A graph in which all the vertices have their degree one of the two values  $\{a, b\}$  is said to be biregular<sup>1</sup>.

#### Definition 6<sup>3</sup>

*Pericondensed benzenoids* constitute Carbon Nanotubes (CNTs), which are ordered in graphite-like, hexagonal pattern. The pericondensed benzenoid graphs  $(r, l)$ ,  $r, l \geq 1$  are obtained by joining  $r$  hexagonal chains with  $l$  hexagons in each chain as seen in Figure 1<sup>3</sup>.

#### Definition 7<sup>3</sup>

A convex benzenoid system has the structure  $BS(n, p, q, r, s)$  for  $n \geq 1, 0 \leq p \leq r \leq n, 0 \leq s \leq q$  and  $p+q = r+s$ . See Figure 2<sup>3</sup>.

#### Definition 8<sup>3</sup>

The convex benzenoid system that reduces according to the component value  $n$ , that is, the parallelogram shaped benzenoid system  $(n, m)$  is depicted in Figure 3<sup>3</sup>.

#### Definition 9<sup>3</sup>

Type –  $IC_4 C_8(S)$  nanosheet  $T'[p, q]$  is the 2-dimensional lattice of  $TUC_4 C_8(S)[p, q]$  nanotube, where  $p$  and  $q$  are defining parameters. See Figures 4 and 53.

#### Definition 10<sup>3</sup>

Type –  $II C_4 C_8(R)$  nanosheet  $T'[p, q]$  is the 2-dimensional lattice of  $TUC_4 C_8(s)[p, q]$  nanotube, where  $p$  and  $q$  are defining parameters. See Figures 6 and 7<sup>3</sup>.

#### Definition 11<sup>3</sup>

A H-naphtalenic nanosheet  $(n, m)$  is made by alternating hexagons  $C_6$ , squares  $C_4$  and octagons  $C_8$ . See Figure 8<sup>3</sup>.

#### Definition 12<sup>6</sup>

The benzenoid system which can be extended to any dimension and satisfies the condition that the limit of the ratio of the number of internal vertices to the total number of vertices is less than 1 as  $n \rightarrow \infty$  are called as homologous series of extruded benzenoid systems. Following are some classes of such graphs. See Figures 9 to 166.

#### Definition 13<sup>11</sup>

The enhanced hypercube  $Q_{r,k}$ ,  $0 \leq k \leq r-1$  is a graph with vertex set same as that of  $Q_r$  and the edge set includes the edges of  $Q_r$  along with the edges between the vertices labelled with complementary indices. See figures 17 and 18<sup>11</sup>.

#### Definition 14<sup>2</sup>

An augmented hypercube is one which the vertex set is same as that of the hypercube with the corresponding dimension. The edges are drawn between the vertices if the binary address denoting the vertices differ exactly by one bit. See figures 19 and 20<sup>2</sup>.

#### Lemma 1<sup>9</sup>

The characteristic polynomial of *Circum-coronene*(1) of the class of chemical graphs *Circum-coronene*( $n$ ) is  $x^6 - 6x^4 + 9x^2 - 4$ .<sup>9</sup>

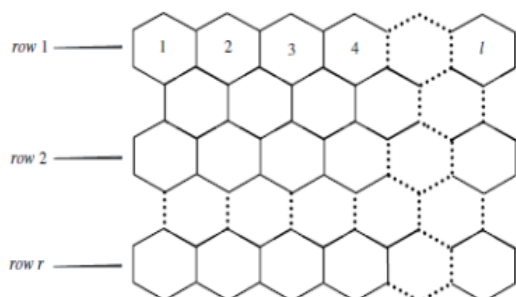
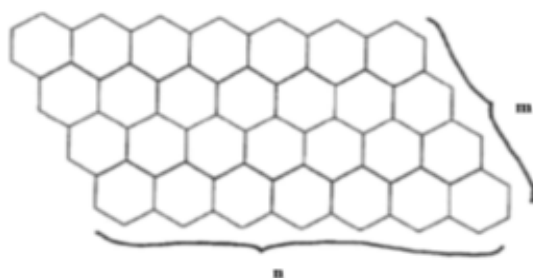
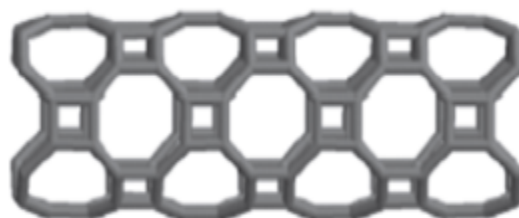
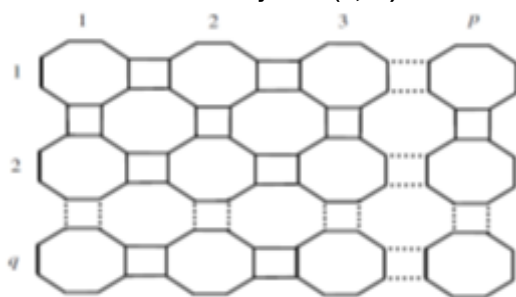
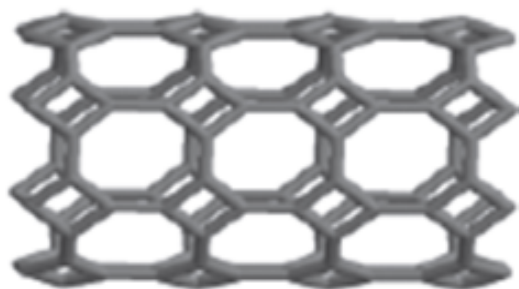
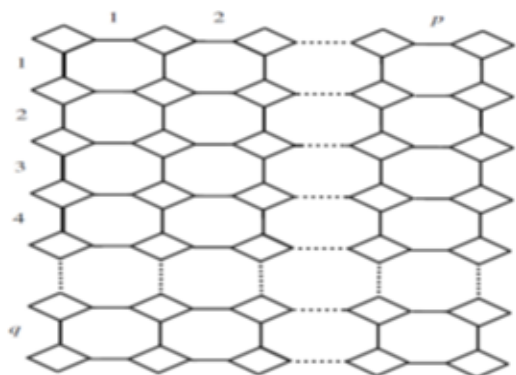
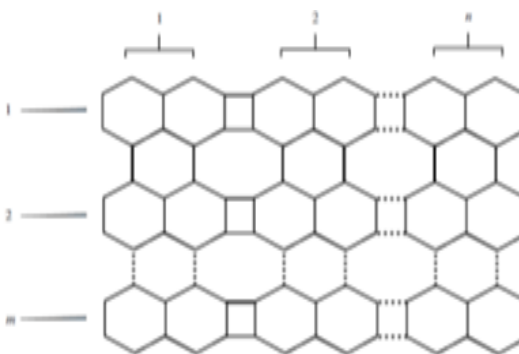
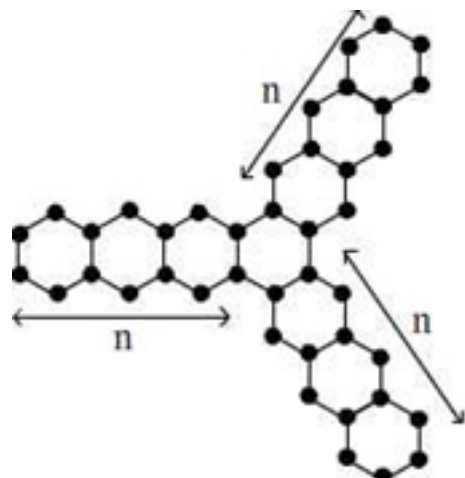
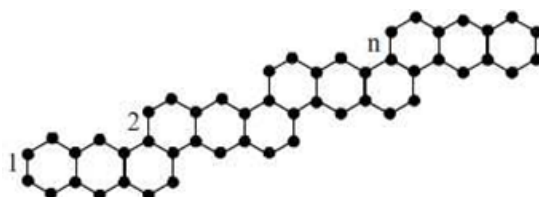
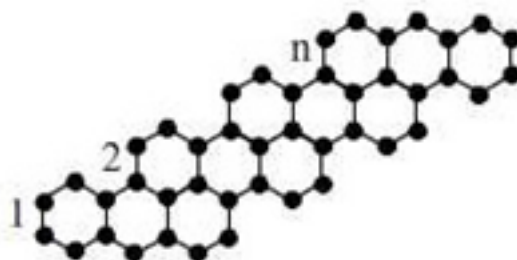
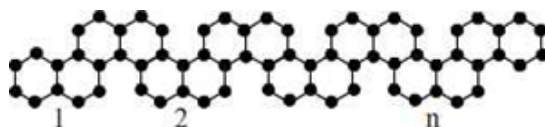
Fig. 1. The pericondensed benzenoid graphs  $(r, l)$ 

Fig. 2. The convex benzenoid system

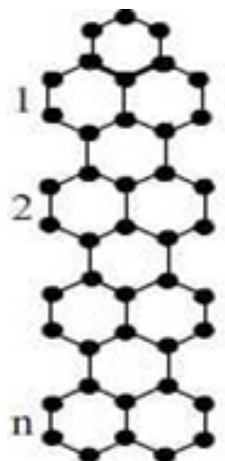
Fig. 3. The parallelogram shaped benzenoid system  $(n, m)$ Fig. 4.  $TUC_4C_8(S)[p,q]$  nanotubeFig. 5. Type – I  $C_4C_8(S)$  nanosheet  $T^{-1}[p,q]$ Fig. 6.  $TUC_4C_8(R)[p,q]$  nanotubeFig. 7. Type – II  $C_4C_8(R)$  nanosheet  $T^2[p,q]$ Fig. 8. H-naphtalenic nanosheet  $(n, m)$

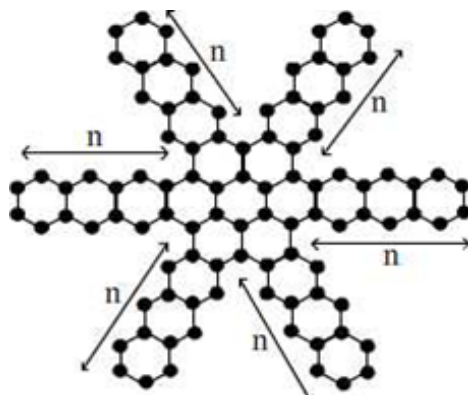
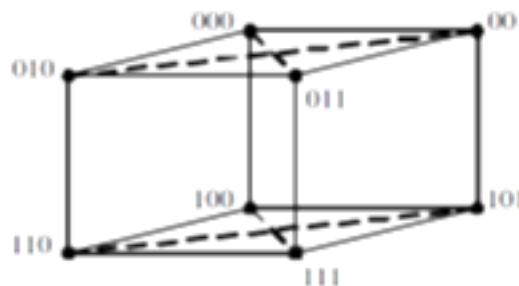
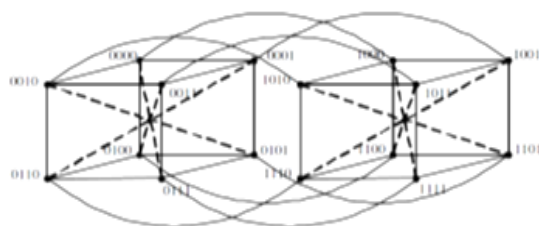
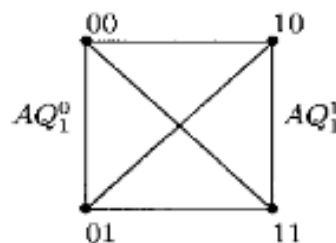
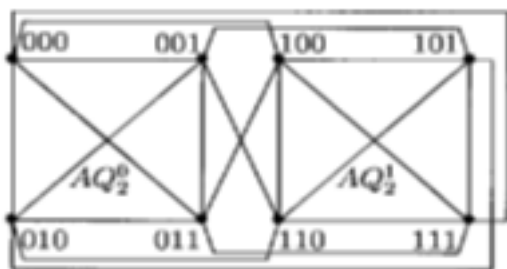
Fig. 9.  $D_n$ Fig. 10.  $E_n$ Fig. 11.  $F_n$ Fig. 12.  $G_n$ **Theorem 1<sup>8</sup>**

If a graph  $G$  is a disconnected graphs with components  $G_1, G_2, \dots, G_k$ , then its characteristic polynomial can be written as a product of the characteristic polynomials of all the components<sup>8</sup>.

**Theorem 2<sup>8</sup>**

If  $uv$  is an edge of  $G$ , then the characteristic

Fig. 13.  $I_n$ Fig. 14.  $J_n$ Fig. 15.  $K_n$

Fig. 16.  $L_n$ Fig. 17.  $Q_{3,2}$ Fig. 18.  $Q_{4,2}$ Fig. 19.  $AQ^2$ Fig. 20.  $AQ^3$ 

polynomial  $\phi(G)$  of the graph  $G$  can be expressed as  $\phi(G) = \phi(G-uv) - \phi(G-u-v) - 2 \sum_{C \in C(uv)} \phi(G-C)$  where  $C(uv)$  is the set of cycles containing  $uv$ .

#### Theorem 3<sup>1</sup>

The largest eigenvalue of the adjacency matrix of a  $k$ -regular graph will be  $k^1$ .

#### Spectral Parameters of Enhanced Hypercube and Augmented Hypercube

#### Theorem 4

The enhanced hypercube  $Q_{r,k}$  has the following spectral parameters:

$$\lambda_1(Q_{r,k}) = \begin{cases} r, & k=0 \\ r+1, & k \geq 1 \end{cases}$$

$$\lambda_2(Q_{r,k}) = \begin{cases} r-2, & k=0,1 \\ r-1, & k \geq 2 \end{cases}$$

$$S_A(Q_{r,k}) = \begin{cases} 3, & k=1 \\ 0, & \text{otherwise} \end{cases}$$

*Proof.* The enhanced hypercubes  $Q_{r,k}$  is a variant of the hypercube with the vertex set same as that of the hypercube and the edge set has some additional edges called complementary edges. All these additional edges which increase the connectivity between the vertices, are incident with one vertex of the form,  $x_0 x_1 x_2 \dots x_{(k-2)} x_{(k-1)} x_k \dots x_{r-1}$  and another vertex of the form  $x_0 x_1 x_2 \dots x_{k-2} x_{k-1} x_k x_{r-1}$ , where  $x_i = 0$  or  $1$ ,  $0 \leq i \leq r-1$ . This  $(r+1)$ -regular graph has  $2^r$  vertices and  $(r+1)2^{r-1}$  edges. Using Theorem 3, (i) follows.

The adjacency matrix of the enhanced

hypercube  $Q_{r,k}$  is a  $2^r \times 2^r$  matrix which can be viewed as  $A + B$ , where  $A$  is the adjacency matrix of the hypercube  $Q_r$  and  $B$  is the adjacency matrix of disjoint copies of some bipartite graphs. When  $r = 2, 3$ , it can be seen that the bipartite graphs are  $P_2$ , when  $r = 4$ , the bipartite graphs are  $C_4$  and so on.

Hence, the matrix  $B$  can in turn be recognized as a sum of adjacency matrices of bipartite graphs. Thus, the adjacency matrix of  $Q_{r,k}$  can be realized as the sum of adjacency matrices of bipartite graphs, since  $Q_r$  is also bipartite. Now, each of these matrices in the sum can be represented in the form of whose spectrum is symmetric with respect to 0.

Thus, solving the characteristic equation of each of these matrices to obtain their eigenvalues would yield the second largest eigenvalue of the adjacency matrix of  $Q_{r,k}$ . Note that all the adjacency matrices considered here are of the order  $2^r \times 2^r$  and only the edges are taken according to the corresponding subgraph. From these formulations, (ii) and (iii) follow.

□

#### Theorem 5

The augmented hypercubes have the following spectral parameters:

$$E(AQ^r) = \begin{cases} 2 & , r = 1 \\ E(AQ^{r-1}) + 4(r-1) & , r \geq 2 \end{cases}$$

$$\lambda_1(AQ^r) = 2r - 1$$

$$\lambda_2(AQ^r) = \begin{cases} 1 & , r = 1 \pmod{2} \\ -1 & , r = 0 \pmod{2} \end{cases}$$

$$\lambda_n(AQ^r) = -2r + 3$$

$$S(AQ^r) = 4(r-1)$$

$$\lambda_1(AQ^r) = \begin{cases} 2n-2, & r = 1 \pmod{2} \\ 2n & , r = 0 \pmod{2} \end{cases}$$

*Proof.* The augmented hypercubes  $AQ^r$  is a variant of the hypercube which has some extra edges apart from those of the hypercube. The vertices are labeled as  $r$ -bit binary strings and the extra edges are between any two distinct vertices if the corresponding elements in the binary string are the same or complement to each other. This resultant

graph which is constructed in a recursive manner is  $2r - 1$  regular and possesses  $2^r$  vertices and  $(2r - 1)2^{r-1}$  edges. Thus, (ii) follows from Theorem 3.

It can be observed that the extra edges that are added form disjoint copies of bipartite graphs such as  $P_2$ ,  $C_4$  and so on. The eigenvalues of the bipartite graphs possess symmetry about zero and can thus be computed in a relatively smaller amount of time compared to other graphs. This ensures that the adjacency matrix of the augmented hypercubes can be realized as the sum of the adjacency matrices of bipartite graphs whose adjacency matrices are represented in the form of a block matrix as shown below:

Note that all the adjacency matrices considered here are of the order  $2^r \times 2^r$  and only the edges are taken according to the corresponding subgraph. Resolving the eigenvalues of the adjacency matrices, the theorem follows.

□

### Spectral Parameters of Pericondensed Benzenoid Graph and Parallelogram Shaped Benzenoid System

#### Theorem 6

The pericondensed benzenoid graph  $(r, l)$  has the following spectral parameters:

$$\text{Energy} \approx 2r(3l+1)$$

$$\text{Spectral Radius} \approx \begin{cases} 2, & \text{if } r = 1 \text{ and } 1 \leq l \leq 4 \\ 3, & \text{otherwise} \end{cases}$$

$$\text{Second largest eigenvalue} \approx \begin{cases} 1, & \text{if } r = 1 \text{ and } l = 1 \\ 2, & \text{if } r = 1 \text{ and } l \geq 2 \\ 2, & \text{if } r = 2 \text{ and } l \leq 4 \\ 3, & \text{otherwise} \end{cases}$$

$$\text{Least eigenvalue} \approx \begin{cases} -2, & \text{if } r = 1 \text{ and } 1 \leq l \leq 4 \\ -3, & \text{otherwise} \end{cases}$$

$$\text{Spread} \approx \begin{cases} 4, & \text{if } r = 1 \text{ and } 1 \leq l \leq 4 \\ 6, & \text{otherwise} \end{cases}$$

$$\text{Separator} \approx \begin{cases} 1, & \text{if } r = 1 \text{ and } l = 1 \\ 1, & \text{if } r = 1 \text{ and } l \geq 5 \\ 1, & \text{if } r = 2 \text{ and } l \leq 4 \\ 0, & \text{otherwise} \end{cases}$$

*Proof.* Pericondensed benzenoid graphs are obtained by attaching  $r$  hexagonal chains of  $l$  hexagons each. See Figure 1. This is a biregular graph which has vertices of degrees 2 and 3 only. One can observe that this is also a bipartite graph whose adjacency matrix can be represented as,

$$\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

in which each partition of the set of vertices possess  $r(2l+1)$  vertices equally.

To obtain the characteristic polynomial, the graph is viewed as  $\frac{l}{2}$  hexagons connected by a path of length 1 or 2. Then, using Lemma 1, the characteristic polynomial of each of these disjoint hexagons can be computed. By Theorem 1, the characteristic polynomial of the disconnected graph in which each of the components is a hexagon can be obtained. Further, considering each of the remaining

$$6r\left(l - \frac{l}{2}\right) + r - l$$

edges that constitute the connecting paths separately and applying Theorem 2, the characteristic polynomial of the pericondensed benzenoid graphs can be achieved from which the theorem follows.

#### Theorem 7

The Parallelogram shaped benzenoid system  $(n, m)$  has the following spectral parameters:

$$\text{Energy} \approx 3m(n+1) + 3n - 1$$

$$\text{Spectral Radius} \approx \begin{cases} 2, & \text{if } m=1 \text{ and } n \leq 5 \\ 2, & \text{if } m \geq 2 \text{ and } n=1 \\ 3, & \text{otherwise} \end{cases}$$

$$\text{Second largest eigenvalue} \approx \begin{cases} 2, & \text{if } m=1 \text{ and } n \leq 5 \\ 2, & \text{if } m=2 \text{ and } n \leq 4 \\ 2, & \text{if } m=3 \text{ and } n \leq 3 \\ 2, & \text{if } m=4 \text{ and } n \leq 2 \\ 2, & \text{if } m=5 \text{ and } n=1 \\ 3, & \text{otherwise} \end{cases}$$

$$\text{Least eigenvalue} \approx \begin{cases} -2, & \text{if } m=1 \text{ and } n \leq 5 \\ -2, & \text{if } m \geq 2 \text{ and } n=1 \\ -3, & \text{otherwise} \end{cases}$$

$$\text{Spread} \approx \begin{cases} 4, & \text{if } m=1 \text{ and } n \leq 5 \\ 4, & \text{if } m \geq 2 \text{ and } n=1 \\ 6, & \text{otherwise} \end{cases}$$

$$\text{Separator} \approx \begin{cases} 1, & \text{if } m=2 \text{ and } n \leq 4 \\ 1, & \text{if } m=3 \text{ and } n \leq 3 \\ 1, & \text{if } m=4 \text{ and } n \leq 2 \\ 0, & \text{otherwise} \end{cases}$$

*Proof.* The parallelogram shaped benzenoid graphs are a class of graphs which possess  $2(mn+m+n)$  vertices. See Figure 3. When  $m$  and  $n$  are equal to 1, it can be seen that its spectrum is, .

$$\begin{pmatrix} -1 & 1 & -2 & 2 \\ 2 & 2 & 1 & 1 \end{pmatrix}$$

Hence, energy is equal to 8 in this case. It can be observed that with increase in one  $m$  value, the number of vertices increase by and with increase in one  $n$  value, the vertices count rise by  $2m+2$ . In each case, the energy increases by  $3n-3$  and  $3m-3$  respectively. Thus, by using mathematical induction, the energy of this class of graph can be obtained as  $3m(n+1)+3n-1$ .

(ii) to (vi) can also be proved in a similar manner.

#### Spectral Parameters of Certain Nanosheets

In this section, the spectral parameters of three nanosheets, namely, Type-I  $C_4C_6(S)$  nanosheet, Type-II  $C_4C_6(R)$  nanosheet, H-naphthalenic nanosheet are obtained by analysing their adjacency matrices.

#### Theorem 8

The Type – I nanosheet, has the following spectral parameters:

$$E(T^1[p, q]) \approx p(12q-1) - q$$

$$\lambda_1(T^1[p, q]) \approx \begin{cases} 2, & \text{if } p=1 \text{ and } q=1 \\ 3, & \text{otherwise} \end{cases}$$

$$\lambda_2(T^1[p, q]) \approx \begin{cases} 1, & \text{if } p=1 \text{ and } q=1 \\ 2, & \text{if } p=1 \text{ and } q=2, 3 \\ 3, & \text{otherwise} \end{cases}$$

$$\lambda_n(T^1[p, q]) \approx \begin{cases} -2, & \text{if } p=1 \text{ and } q=1 \\ -3, & \text{otherwise} \end{cases}$$

$$S(T^1[p, q]) \approx \begin{cases} 4, & \text{if } p=1 \text{ and } q=1 \\ 6, & \text{otherwise} \end{cases}$$

$$S_A(T^1[p, q]) \approx \begin{cases} 1, & \text{if } p=1 \text{ and } 1 \leq q \leq 3 \\ 0, & \text{otherwise} \end{cases}$$

*Proof.* The Type-I  $C_4C_8(S)$  nanosheet  $T^1[p, q]$  is a tessellation of  $C_8$  connected by adjoining the cycle  $C_4$ . See Figure 5. The adjacency matrix of this class of graphs is a  $8pq \times 8pq$  matrix that can be represented as the sum of adjacency matrix of the disjoint components of  $C_8$  and the adjacency matrix of the disjoint components of  $C_4$ . Both these adjacency matrices are of the form

$$\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

since the components of  $C_8$  and  $C_4$  are bipartite. The characteristic polynomial of these components of and can be obtained as an outcome of Theorem 1. Note that the adjacency matrices considered here are of order  $8pq \times 8pq$  and only the edges are taken according to the corresponding subgraph. With these formulations, the characteristic polynomial for this class of graph can be easily obtained and hence the theorem follows.

□

**Remark 1**  $E(T^1[p, q]) = E(T^1[q, p])$

#### Theorem 9

The Type-II  $C_4C_8(R)$  nanosheet, denoted by  $T^2[p, q]$  has the following spectral parameters:

$$\begin{aligned} E(T^2[p, q]) &\approx 5pq + 6(p + q) + 4 \\ \lambda_1(T^2[p, q]) &\approx 3 \\ \lambda_2(T^2[p, q]) &\approx \begin{cases} 2, & \text{if } p = 1 \text{ and } q = 1, 2 \\ 3, & \text{otherwise} \end{cases} \\ \lambda_n(T^2[p, q]) &\approx -3 \\ S(T^2[p, q]) &\approx 6 \\ S_A(T^2[p, q]) &\approx \begin{cases} 1, & \text{if } p = 1 \text{ and } q = 1, 2 \\ 0, & \text{otherwise} \end{cases} \end{aligned}$$

*Proof.* The Type-II  $C_4C_8(R)$  nanosheet is a trivalent decoration which consists of the cycles  $C_4$  connected to one another by a single edge. See Figure 7. This forms a tessellation of  $C_4$  and  $C_8$ . The adjacency matrix for this class of graphs will

be a  $4(p+1)(q+1) \times 4(p+1)(q+1)$  matrix which can be realised as the sum of adjacency matrices of disjoint components of  $C_4$  and  $C_8$ . Now, the characteristic polynomial of the disjoint components of and can be computed as an outcome of Theorem 1. From these formulations, one can easily obtain the characteristic polynomial for this class of graph and hence the theorem follows

**Remark 2.**  $T^2[p, q] = E(T^2[q, p])$

**Theorem 10.** The  $H$ -naphtalenic nanosheet  $(n, m)$  has the following spectral parameters:

$$\begin{aligned} \text{Energy} &\approx 2[n(8m-1) - (m-1)] \\ \text{Spectral radius} &\approx \begin{cases} 2, & \text{if } n = 1 \text{ and } m = 1 \\ 3, & \text{otherwise} \end{cases} \\ \text{Second largest eigenvalue} &\approx \begin{cases} -2, & \text{if } n = 1 \text{ and } m = 1 \\ -3, & \text{otherwise} \end{cases} \\ \text{Least eigenvalue} &\approx \begin{cases} -2, & \text{if } n = 1 \text{ and } m = 1 \\ -3, & \text{otherwise} \end{cases} \\ \text{Spread} &\approx \begin{cases} 4, & \text{if } n = 1 \text{ and } m = 1 \\ 6, & \text{otherwise} \end{cases} \\ \text{Separator} &\approx \begin{cases} 1, & \text{if } n = 1 \text{ and } m = 2 \\ 0, & \text{otherwise} \end{cases} \end{aligned}$$

*Proof.* The class of  $H$ -naphtalenic nanosheet is a class of graphs which constitutes the cycles  $C_4$ ,  $C_6$  and  $C_8$ . This is a trivalent decoration which consists of  $m$  chains containing  $n$  pairs of hexagons connected by  $C_4$ . See Figure 8. Adjoining these chains by connecting the vertices of hexagons together, an octagon is formed. The adjacency matrix for this class of graph is  $10mn \times 10mn$  matrix that can be represented as the sum of three adjacency matrices of the hexagons, squares and octagons respectively. Note that all the adjacency matrices considered here are of the order  $10mn \times 10mn$  and only the edges are taken according to the corresponding subgraph namely, hexagons, squares and octagons. The characteristic polynomial of each of these adjacency matrices which constitute the sum may be computed using Theorem 1. With these formulations, one can easily obtain the characteristic polynomial for this class of graphs and hence the theorem follows.

□



### Spectral parameters of the homologous series of extruded benzenoid systems

This section includes the findings on the spectral parameters of some homologous series of extruded benzenoid systems which extend with respect to one parameter.

#### Theorem 11

The benzenoid system  $D_n$ , given in Figure 9, has the following spectral parameters:

$$E(D_n) \approx 17n + 8$$

$$\lambda_1(D_n) = 3$$

$$\lambda_2(D_n) = \begin{cases} 2, & \text{if } n \leq 3 \\ 3, & \text{if } n \geq 4 \end{cases}$$

$$\lambda_n(D_n) = -3$$

$$S(D_n) = 6$$

$$S_A(D_n) = \begin{cases} 1, & \text{if } n \leq 3 \\ 0, & \text{if } n \geq 4 \end{cases}$$

*Proof.* The benzenoid system  $D_n$  is a class of graphs that extends in three directions for one dimension. The total number of vertices in each dimension is  $12n+6$ . For  $n=0$ , it follows from Lemma 1 that the spectrum of  $D_n$  is

$$\begin{pmatrix} -1 & 1 & -2 & 2 \\ 2 & 2 & 1 & 1 \end{pmatrix}$$

and hence  $E(D_0)=8$ . As the dimension of increases by one, the vertices count increase by 12 and the value of energy increases by 17 (approx.). Using mathematical induction, it follows that  $E(D_n)=17n+8$ . (ii) to (vi) can be proved in a similar manner.  $\square$

#### Theorem 12

The benzenoid system  $E_n$ , given in Figure 10, has the following spectral parameters:

*Proof.* The benzenoid system  $E_n$  extends in each dimension with the attachment of three hexagons to the graph of preceding dimension. See Figure 10. The total number of vertices for this class of graph

$$E(E_n) \approx 17n + 2$$

$$\lambda_1(E_n) = \begin{cases} 2, & \text{if } n = 1 \\ 3, & \text{if } n \geq 2 \end{cases}$$

$$\lambda_2(E_n) = \begin{cases} 2, & \text{if } n \leq 2 \\ 3, & \text{if } n \geq 3 \end{cases}$$

$$\lambda_n(E_n) = \begin{cases} -2, & \text{if } n = 1 \\ -3, & \text{if } n \geq 2 \end{cases}$$

$$S(E_n) = \begin{cases} 4, & \text{if } n = 1 \\ 6, & \text{if } n \geq 2 \end{cases}$$

$$S_A(E_n) = \begin{cases} 1, & \text{if } n = 2 \\ 0, & \text{otherwise} \end{cases}$$

is  $12n+2$ . The number of vertices increase by 12 for increase in one dimension which in turn increases the energy by 19 (approx.). Using mathematical induction, it is clear that  $E(E_n)=17n+2$ . Similarly, (ii) to (vi) can be proved.  $\square$

#### Theorem 13

The benzenoid system, given in Figure 11, has the following spectral parameters:

*Proof.* The benzenoid system  $F_n$  is a class of graphs that possesses  $10n+4$  vertices which extends by appending three hexagons to the graph of the preceding dimension. It can be observed that the vertices count increase by 10 and the value of energy increases by 25 (approx.) with increase in one dimension. Using mathematical induction, one can see that  $E(F_n)=15n+4$ . (ii) to (vi) can be proved

$$E(F_n) \approx 15n + 4$$

$$\lambda_1(F_n) = \begin{cases} 2, & \text{if } n = 1 \\ 3, & \text{if } n \geq 2 \end{cases}$$

$$\lambda_2(F_n) = \begin{cases} 2, & \text{if } n \leq 2 \\ 3, & \text{if } n \geq 3 \end{cases}$$

$$\begin{aligned}
 {}_n \left( \begin{array}{c} n \\ n \end{array} \right) &= \begin{cases} -2, & \text{if } n = 1 \\ -3, & \text{if } n \geq 2 \end{cases} \\
 \left( \begin{array}{c} n \\ n \end{array} \right) &= \begin{cases} 4, & \text{if } n = 1 \\ 6, & \text{if } n \geq 2 \end{cases} \\
 S_A(F_n) &= \begin{cases} 1, & \text{if } n = 2 \\ 0, & \text{otherwise} \end{cases}
 \end{aligned}$$

in a similar manner. Along similar lines, we prove the following results.

**Theorem 14**

The benzenoid system  $G_n$ , given in Figure 12, has the following spectral parameters:

**Theorem 15**

The benzenoid system  $\Pi_n$ , given in Figure 13, has the following spectral parameters:

**Theorem 16**

The benzenoid system  $J_n$ , given in Figure 14, has the following spectral parameters:

**Theorem 17**

The benzenoid system  $K_n$ , given in Figure 15, has the following spectral parameters:

**Theorem 18**

The benzenoid system  $L_n$ , given in Figure 16, has the following spectral parameters:

$$\begin{aligned}
 E(G_n) &\approx 23n + 2 \\
 \lambda_1(G_n) &= 3 \\
 \lambda_2(G_n) &= \begin{cases} 2, & \text{if } n = 1 \\ 3, & \text{if } n \geq 2 \end{cases} \\
 \lambda_n(G_n) &= -3 \\
 S(G_n) &= 6 \\
 S_A(G_n) &= \begin{cases} 1, & \text{if } n = 1 \\ 0, & \text{if } n \geq 2 \end{cases}
 \end{aligned}$$

$$\begin{aligned}
 E(\mathbb{I}_n) &\approx 14n \\
 \lambda_1(\mathbb{I}_n) &= \begin{cases} 2, & \text{if } n = 1 \\ 3, & \text{if } n \geq 2 \end{cases} \\
 \lambda_2(\mathbb{I}_n) &= \begin{cases} 2, & \text{if } n \leq 3 \\ 3, & \text{if } n \geq 4 \end{cases} \\
 \lambda_n(\mathbb{I}_n) &= \begin{cases} -2, & \text{if } n = 1 \\ -3, & \text{if } n \geq 2 \end{cases} \\
 S(\mathbb{I}_n) &= \begin{cases} 4, & \text{if } n = 1 \\ 6, & \text{if } n \geq 2 \end{cases} \\
 S_A(\mathbb{I}_n) &= \begin{cases} 1, & \text{if } n = 2, 3 \\ 0, & \text{otherwise} \end{cases}
 \end{aligned}$$

$$E(J_n) \approx 15n + 3$$

$$\lambda_1(J_n) = \begin{cases} 2, & \text{if } n = 1 \\ 3, & \text{if } n \geq 2 \end{cases}$$

$$\lambda_2(J_n) = \begin{cases} 2, & \text{if } n \leq 2 \\ 3, & \text{if } n \geq 3 \end{cases}$$

$$\lambda_n(J_n) = \begin{cases} -2, & \text{if } n = 1 \\ -3, & \text{if } n \geq 2 \end{cases}$$

$$S(J_n) = \begin{cases} 4, & \text{if } n = 1 \\ 6, & \text{if } n \geq 2 \end{cases}$$

$$S_A(J_n) = \begin{cases} 1, & \text{if } n = 2 \\ 0, & \text{otherwise} \end{cases}$$

$$E(\mathbb{K}_n) \approx 15n + 8$$

$$\lambda_1(\mathbb{K}_n) = 3$$

$$\lambda_2(\mathbb{K}_n) = \begin{cases} 2, & \text{if } n \leq 2 \\ 3, & \text{if } n \geq 3 \end{cases}$$

$$\lambda_n(\mathbb{K}_n) = -3$$

$$S(\mathbb{K}_n) = 6$$

$$S_A(\mathbb{K}_n) = \begin{cases} 1, & \text{if } n \leq 2 \\ 0, & \text{otherwise} \end{cases}$$

$$E(L_n) \approx 34n + 35$$

$$\lambda_1(L_n) = 3$$

$$\lambda_2(L_n) = 3$$

$$\lambda_n(L_n) = -3$$

$$S(L_n) = 6$$

$$S_A(L_n) = 0$$

## CONCLUSION

The various chemical structures considered in this article have vast practical applications. With the motive of obtaining the quantum-theoretic characteristics of these molecules, some spectral parameters are computed for the same. In particular, analytic expressions have been derived for different spectral parameters of various classes of chemical graphs. It is also observed that energy increases with increase in dimension for all the chemical graphs considered. Further, the results obtained in this article verify the fact that all molecular graphs are non-hyperenergetic. We believe that the results obtained in this article will pave way for a cost effective, time saving interpretations about chemical graphs and interconnection networks.

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