Armenian Journal of Mathematics
Volume 15, Number 10, 2023, 1–16
https://doi.org/10.52737/18291163-2023.15.10-1-16

On the Distance Spectrum and Distance-Based Topological Indices of Central Vertex-Edge Join of Three Graphs

T. Haritha and A.V. Chithra

Abstract. In this paper, we introduce a new graph operation based on a central graph called central vertex-edge join (denoted by $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$) and then determine the distance spectrum of $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$ in terms of the adjacency spectra of regular graphs G_1, G_2 and G_3 when G_1 is triangle-free. As a consequence of this result, we construct new families of non-D-cospectral D-equienergetic graphs. Moreover, we determine bounds for the distance spectral radius and distance energy of the central vertex-edge join of three regular graphs. In addition, we provide its results related to graph invariants like eccentric-connectivity index, connective eccentricity index, total-eccentricity index, average eccentricity index, Zagreb eccentricity indices, eccentric geometric-arithmetic index, eccentric atom-bond connectivity index, Wiener index. Using these results, we calculate the topological indices of the organic compounds Methylcyclobutane (C_5H_{10}) and Spirohexane (C_6H_{10}).

Key Words: Distance Matrix, Distance Eigenvalues, Distance Equienergetic Graphs, Topological Indices
Mathematics Subject Classification 2020: 05C50, 05C76, 05C12

Introduction

We start with the necessary definitions and notations. All graphs considered in this paper are simple connected and undirected. Let $G_n = (V(G_n), E(G_n))$ be a graph of order n and size m, with vertices v_i, $1 \leq i \leq n$ and edges e_j, $1 \leq j \leq m$. The *adjacency matrix* of a graph G_n is a square symmetric matrix $A(G_n) = (a_{ij})_{n\times n}$, where $a_{ij} = 1$ when v_i is adjacent to v_j and $a_{ij} = 0$ otherwise. Denote the eigenvalues of $A(G_n)$ (A-eigenvalues) by $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$, then the collection of all the eigenvalues of $A(G_n)$ is said to be the adjacency spectrum of G_n. The *incidence matrix* of a graph G_n is the $n \times m$ matrix $Q(G_n) = (q_{ij})_{n\times m}$, where $q_{ij} = 1$ when v_i is incident to e_j and $q_{ij} = 0$ otherwise. The *line graph* $L(G_n)$ of G_n is a graph with $V(L(G_n)) = E(G_n)$ such that two vertices in $L(G_n)$ are adjacent only if the corresponding edges in G_n have an end vertex in common. For a partitioned matrix, we denote its *equitable quotient matrix* by M [3] and all one entry matrix by $J_{n\times m}$. We denote by C_n the *cycle*, by $K_{p,q}$ $(p + q = n)$ the *complete bipartite graph*, and by K_n the *complete graph* each of order n.

The *distance* $d_{G_n}(v_i, v_j)$ between two vertices is the length of the shortest path connecting them in G_n [4]. In particular, $d_{G_n}(v_i, v_i) = 0$, for any $v_i \in V(G_n)$. The eccentricity of a vertex $v_i \in V(G_n)$ is defined as $ec_{G_n}(v_i) = max\{d(v_i, v_j) : v_j \in V(G_n)\}$. The square symmetric matrix $D(G_n) = (d_{ij})_{n\times n} = d_{G_n}(v_i, v_j)$ is called the *distance matrix* of G_n and its eigenvalues are said to be the distance eigenvalues (D-eigenvalues). Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_t$ be the distinct D-eigenvalues of G_n with multiplicities $s_1, s_2, \ldots, s_t$. Then the *distance spectrum*(D-spectrum) of G_n is given by

$$Spec_D(G_n) = \begin{pmatrix} \mu_1 & \mu_2 & \ldots & \mu_t \\ s_1 & s_2 & \ldots & s_t \end{pmatrix}.$$

The D-eigenvalue, $\mu_1(G_n)$, is called the distance spectral radius of G_n. The non-isomorphic graphs of the same order having identical D-spectrum are called *D-cospectral graphs.* The *transmission* $Tr(v_i)$ of a vertex v_i is the sum of all distances from v_i to all other vertices in G. See [2] for a survey of the distance spectra of graphs.

In graph theory, operations on graphs play a significant role. For significant works on distance spectra of graph operations, see [1, 12, 14]. The *central graph* $C(G_n)$ of G_n [20], is the graph obtained by adding new vertex to each edge of G_n and joining all the non adjacent vertices in G_n. In [16], the authors defined the central vertex (edge) join of two graphs and their adjacency spectra are investigated when G_{n_1} and G_{n_2} are both regular graphs. Inspired by these works, we introduce a new graph operation based on central graph and join.

Definition 1 *Let G_{n_1}, G_{n_2} and G_{n_3} be any three graphs of orders n_1, n_2, n_3 and sizes m_1, m_2, m_3, respectively. The central vertex-edge join (CVE-join) of G_{n_1} with G_{n_2} and G_{n_3} is the graph $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$, which is obtained from $C(G_{n_1})$, G_{n_2} and G_{n_3} by joining each vertex of G_{n_1} with every vertex of G_{n_2} and each vertex corresponding to the edges of G_{n_1} with every vertex of G_{n_3}. The set of vertices in $C(G_{n_1})$ corresponding to the edges of G_{n_1} is denoted by $I(G_{n_1})$ (see Fig. 1).*

The order and size of $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$ are $n_1 + m_1 + n_2 + n_3$ and $m_1 + m_2 + m_3 + n_1n_2 + m_1n_3 + (n_1^2 - n_1)/2$, respectively.

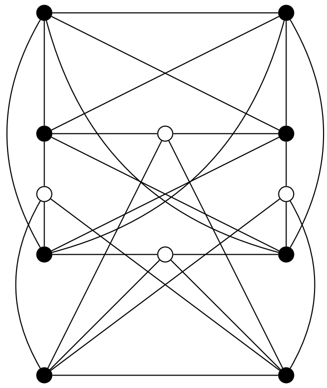

Figure 1: $C_4^C \triangleright (K_2^V \cup K_2^E)$.

In general, finding the D-spectrum of complicated networks is a difficult problem. In Section 2, we obtain the D-spectrum of CVE-join of three regular graphs. Using this we can find the D-spectra of more complicated networks.

The *distance energy* (D-energy) was introduced by Indulal et al. [15], and it is defined as the sum of absolute values of D-eigenvalues of G_n, denoted by $E_D(G_n)$. Two graphs of the same order having equal D-energy are called *D-equienergetic graphs*. In the literature [13, 17, 12], we can see the constructions of different D-equienergetic graphs. In Section 2, using the above operation we provide a new class of D-equienergetic graphs of diameter 3.

The study of graphs through their topological descriptors is beneficial for deriving their underlying topologies. This process has many applications in modeling physico-chemical properties of molecules by QSARs/QSPRs (quantitative structure-activity relationships/quantitative structure-property relationships) analysis. In the studies of QSARs and QSPRs, the topological descriptors of graphs are used to approximate the biological activities and properties of chemical compounds. Various topological indices of chemical structures have emerged as a result of successful applications of QSAR/QSPR studies. This article gives some distance-based topological indices of the new graph operation central vertex-edge join of three graphs.

The following are some graph parameters which are in terms of vertex degrees, eccentricity and distance of a graph G_n.

The *eccentric connectivity index* of G_n is introduced in [18] as

$$\xi^c(G_n) = \sum_{v_i \in V(G_n)} deg_{G_n}(v_i) ec_{G_n}(v_i). \tag{1}$$

The *connective eccentricity index* [11] of G_n is

$$\xi^{ce}(G_n) = \sum_{v_i \in V(G_n)} \frac{deg_{G_n}(v_i)}{ec_{G_n}(v_i)}. \tag{2}$$

By using the eccentric connectivity index, the *total-eccentricity index* [8] is given by

$$\tau(G_n) = \sum_{v_i \in V(G_n)} ec_{G_n}(v_i). \tag{3}$$

The mean value of eccentricity of vertices in $V(G_n)$ is called the *average eccentricity* [19]

$$aveg(G_n) = \frac{1}{n} \sum_{v_i \in V(G_n)} ec_{G_n}(v_i) = \frac{\tau(G_n)}{n}. \tag{4}$$

The *Zagreb indices* [9] of G_n in terms of eccentricities are

$$\begin{aligned} M_1(G_n) &= \sum_{v_i \in V(G_n)} ec^2_{G_n}(v_i), \\ M_2(G_n) &= \sum_{v_i v_j \in E(G_n)} ec_{G_n}(v_i) ec_{G_n}(v_j). \end{aligned} \tag{5}$$

The *geometric-arithmetic index* [10] in terms of eccentricity is given by

$$GA_4(G_n) = \sum_{v_i v_j \in E(G_n)} \frac{2\sqrt{ec_{G_n}(v_i) ec_{G_n}(v_j)}}{ec_{G_n}(v_i) + ec_{G_n}(v_j)}. \tag{6}$$

The *atom-bond connectivity index* [7] in terms of eccentricity is given by

$$ABC_5(G_n) = \sum_{v_i v_j \in E(G_n)} \sqrt{\frac{ec_{G_n}(v_i) + ec_{G_n}(v_j) - 2}{ec_{G_n}(v_i) ec_{G_n}(v_j)}}. \tag{7}$$

The *Wiener index* $W(G)$ [21] of G_n is defined as

$$W(G_n) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_G(v_i, v_j) = \frac{1}{2} \sum_{v_i \in V(G_n)} Tr(v_i). \tag{8}$$

Section 3 gives all the mentioned above indices of central vertex-edge join of three graphs. As a consequence of these results, we calculate different topological indices of the organic compounds Methylcyclobutane (C_5H_{10}) and Spirohexane (C_6H_{10}). Also, we obtain bounds for the distance spectral radius and distance energy of the central vertex-edge join of three graphs.

1 Distance spectrum of CVE-join of three regular graphs

In this section, we discuss the D-spectrum of $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$, where G_{n_1} is a triangle-free regular graph and G_{n_2}, G_{n_3} are two regular graphs.

Lemma 1 *[5] Let G_n be a k-regular graph of order n and size m with $Spec(G_n) = \{\theta_1, \theta_2, \ldots, \theta_n\}$. Then*

$$Spec(L(G_n)) = \begin{pmatrix} 2k-2 & \theta_2+k-2 & \ldots & \theta_n+k-2 & -2 \\ 1 & 1 & \ldots & 1 & m-n \end{pmatrix}.$$

Moreover, -2 is an eigenvalue of $L(G_n)$ with eigenvector V if and only if $Q(G_n)V = 0$.

Theorem 1 *For $i = 1, 2, 3$, let $k_i = \theta_{i1} \geq \theta_{i2} \geq \cdots \geq \theta_{in_i}$ be the A-eigenvalues of the k_i-regular graph G_{n_i} of order n_i and size m_i, where G_{n_1} is triangle-free. Then the D-eigenvalues of $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$ are the following:*
(i) $(-3+\theta_{1j} \pm \sqrt{(\theta_{1j}+1)^2+4(\theta_{1j}+k_1)})/2$, $j = 2, 3, \ldots, n_1$;
(ii) -2 with multiplicity $m_1 - n_1$;
(iii) $-\theta_{ij} - 2$, $i = 2, 3$ and $j = 2, 3, \ldots, n_i$;
(iv) eigenvalues of the matrix

$$\begin{bmatrix} n_1-1+k_1 & 2m_1-k_1 & n_2 & 2n_3 \\ 2n_1-2 & 2m_1-2 & 2n_2 & n_3 \\ n_1 & 2m_1 & 2n_2-k_2-2 & 3n_3 \\ 2n_1 & m_1 & 3n_2 & 2n_3-k_3-2 \end{bmatrix}.$$

Proof. By a proper ordering of vertices in $G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$, the distance matrix $D(G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3}))$ can be written as

$$\begin{bmatrix} J-I+A(G_{n_1}) & 2J-Q(G_{n_1}) & J & 2J \\ 2J-Q(G_{n_1})^T & 2(J-I) & 2J & J \\ J & 2J & 2(J-I)-A(G_{n_2}) & 3J \\ 2J & J & 3J & 2(J-I)-A(G_{n_3}) \end{bmatrix}.$$

Let $k_i = \theta_{i1} \geq \theta_{i2} \geq \cdots \geq \theta_{in_i}$ be the A-eigenvalues of G_{n_i}, where $i = 1, 2, 3$. Let U be a vector such that $A(G_{n_1})U = \theta_{1j}U$ for $j = 2, 3, \ldots, n_1$, then by Perron-Frobenius theory, we have $J_{1\times n_1}U = 0$.

Now, let $\phi_1 = \begin{bmatrix} tU & Q(G_{n_1})^TU & 0 & 0 \end{bmatrix}^T$ be an eigenvector of $D(G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3}))$ for the eigenvalue μ, where t is a real number. Then $D(G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3}))\phi_1 = \mu\phi_1$. That is,

$$\begin{bmatrix} J-I+A(G_{n_1}) & 2J-Q(G_{n_1}) & J & 2J \\ 2J-Q(G_{n_1})^T & 2(J-I) & 2J & J \\ J & 2J & 2(J-I)-A(G_{n_2}) & 3J \\ 2J & J & 3J & 2(J-I)-A(G_{n_3}) \end{bmatrix}\phi_1$$
$$= \mu\phi_1,$$

$$\begin{bmatrix} (-t+\theta_{1j}t-\theta_{1j}-k_1)U \\ (-t-2)Q(G_{n_1})^TU \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \mu tU \\ \mu Q(G_{n_1})^TU \\ 0 \\ 0 \end{bmatrix}.$$

Therefore,

$$\begin{aligned} -t+\theta_{1j}t-\theta_{1j}-k_1 &= \mu t,\\ -t-2 &= \mu,\\ t^2+(\theta_{1j}+1)t-(\theta_{1j}+k_1) &= 0,\\ t_1 &= \frac{-(\theta_{1j}+1)+\sqrt{(\theta_{1j}+1)^2+4(\theta_{1j}+k_1)}}{2},\\ t_2 &= \frac{-(\theta_{1j}+1)-\sqrt{(\theta_{1j}+1)^2+4(\theta_{1j}+k_1)}}{2}. \end{aligned}$$

That is, $-t_1-2$ and $-t_2-2$ are eigenvalues of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$ corresponding to the eigenvalues $\theta_{1j}\neq k_1$ of $A(G_{n_1})$. Thus, we get $2(n_1-1)$ eigenvalues of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$.

By Lemma 1, $Q(G_{n_1})V=0$, where V is an eigenvector of $L(G_{n_1})$ corresponding to the eigenvalue -2 (repeated m_1-n_1 times).

If $\phi_2=\begin{bmatrix}0 & V & 0 & 0\end{bmatrix}^T$, then $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))\phi_2=-2\phi_2$. Therefore, -2 is an eigenvalue of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$ repeated m_1-n_1 times.

Consider the eigenvalue θ_{2j} (for $j=2,3,\ldots,n_2$) of G_{n_2} with an eigenvector W such that $J_{1\times n_2}W=0$. Put $\phi_3=\begin{bmatrix}0 & 0 & W & 0\end{bmatrix}^T$, then $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))\phi_3=-(\theta_{2j}+2)\phi_3$. This shows that $-(\theta_{2j}+2)$, $j=2,3,\ldots,n_2$ are eigenvalues of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$ corresponding to the eigenvalues $\theta_{2j}\neq k_2$ of $A(G_{n_2})$.

Similarly, for each eigenvalue θ_{3j} (for $j=2,3,\ldots,n_3$) of G_{n_3}, we get an eigenvalue $-(\theta_{3j}+2)$ of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$ with eigenvector $\begin{bmatrix}0 & 0 & 0 & X\end{bmatrix}^T$. Thus, we have $2n_1-2+m_1-n_1+n_2-1+n_3-1=n_1+m_1+n_2+n_3-4$ eigenvalues of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$. All the other eigenvalues of $D(G^C_{n_1}\rhd(G^V_{n_2}\cup G^E_{n_3}))$ are the eigenvalues of the equitable quotient matrix

$$M=\begin{bmatrix} n_1-1+k_1 & 2m_1-k_1 & n_2 & 2n_3\\ 2n_1-2 & 2m_1-2 & 2n_2 & n_3\\ n_1 & 2m_1 & 2n_2-k_2-2 & 3n_3\\ 2n_1 & m_1 & 3n_2 & 2n_3-k_3-2 \end{bmatrix}.$$

□

Using Theorem 1, we present some new families of D-equienergetic graphs.

A partition of a nonnegative integer a is a representation of a as a sum of positive integers, called summands or parts of the partition. For a fixed $a\in\mathbb{N}$, let $\mathcal{P}_a$ be the family of all partitions of a, denoted by $p_1,p_2,\ldots,p_s$, each of size at least 3. For $P=\{p_1,p_2,\ldots,p_s\}\in\mathcal{P}_a$, let C_P be the union of cycles with vertices $p_1,p_2,\ldots,p_s$. Then, the order of C_P is a.

Theorem 2 *Let H_{n_1} be a k_1-regular triangle free graph of order n_1 and size m_1 and H_{n_2} be a k_2- regular graph of order n_2 and size m_2 with the least eigenvalue being at least -2. Then, for fixed $a\in\mathbb{N}$ and every partition of $'a'$, $H^C_{n_1}\rhd(C^V_P\cup H^E_{n_2})$ forms a family of D-equienergetic graphs.*

Proof. Let $k_1 = \theta_1 \geq \theta_2 \geq \cdots \geq \theta_{n_1}$, $2 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_a$ and $k_2 = \gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_{n_2}$ be the A-eigenvalues of H_{n_1}, C_P and H_{n_2}, respectively. From Theorem 1, it follows that for every partition P of a the D-eigenvalues of $H^C_{n_1} \triangleright (C^V_P \cup H^E_{n_2})$ are $\left(-3+\theta_j \pm \sqrt{(\theta_j+1)^2+4(\theta_j+k_1)}\right)/2$, $j = 2, 3, \ldots, n_1$; -2 with multiplicity $m_1 - n_1$; $-\lambda_{j'} - 2$, $j' = 2, 3, \ldots, a$; $-\gamma_{j''} - 2, j'' = 2, 3, \ldots, n_2$ and the eigenvalues of the equitable quotient matrix M of $H^C_{n_1} \triangleright (C^V_P \cup H^E_{n_2})$

$$M = \begin{bmatrix} n_1+k_1-1 & 2m_1-k_1 & a & 2n_2 \\ 2n_1-2 & 2m_1-2 & 2a & n_2 \\ n_1 & 2m_1 & 2a-4 & 3n_2 \\ 2n_1 & m_1 & 3a & 2n_2-k_2-2 \end{bmatrix}.$$

Since $\lambda_{j'} \geq -2$ for $j' = 2, 3, \ldots, a$, we have $-(\lambda_{j'}+2) \leq 0$. Similarly, $-(\gamma_{j''}+2) \leq 0, j'' = 2, 3, \ldots, n_2$. Therefore,

$$\begin{aligned}\sum_{j'=2}^{a}|-\lambda_{j'}-2| + \sum_{j''=2}^{n_2}|-\gamma_{j''}-2| &= \sum_{j'=2}^{a}(\lambda_{j'}+2) + \sum_{j''=2}^{n_2}(\gamma_{j''}+2) \\ &= -2+2(a-1)-k_2+2(n_2-1) \\ &= 2a-k_2+2n_2-6.\end{aligned}$$

Hence, for every partition of a, the energy remains the same. □

2 Distance-based topological indices of CVE-join of three graphs

This section gives various distance-based topological indices of the central vertex-edge join of three graphs. The following well-known theorems are used in the main results.

Theorem 3 *[22] Let G_n be a connected graph with $n \geq 2$. Then*

$$\mu_1(G_n) \geq \frac{2}{n} W(G_n).$$

with equality if and only if the row sums of $D(G_n)$ are all equal.

Theorem 4 *[6] Let G_n be a connected graph with diameter d. Then*

$$E_D(G_n) \leq \sqrt{2n}\left((2-\sqrt{2})d + (\sqrt{2}-1)W(G_n)\right).$$

For three graphs G_{n_1}, G_{n_2} and G_{n_3}, their CVE-join $\mathcal{G} = G_{n_1}^C \triangleright (G_{n_2}^V \cup G_{n_3}^E)$ has the following properties:

$$deg_{\mathcal{G}}(v) = \begin{cases} n_1 + n_2 - 1 & \text{if } v \in V(G_{n_1}), \\ n_3 + 2 & \text{if } v \in I(G_{n_1}), \\ deg_{G_{n_2}}(v) + n_1 & \text{if } v \in V(G_{n_2}), \\ deg_{G_{n_3}}(v) + m_1 & \text{if } v \in V(G_{n_3}). \end{cases} \tag{9}$$

Now we give the eccentricity of vertices in $\mathcal{G}$ by two different cases.
Case 1. If G_{n_1} is a triangle free graph,

$$ec_{\mathcal{G}}(v) = \begin{cases} 2 & \text{if } v \in V(G_{n_1}) \text{ or } v \in I(G_{n_1}), \\ 3 & \text{if } v \in V(G_{n_2}) \text{ or } v \in V(G_{n_3}). \end{cases} \tag{10}$$

Case 2. If G_{n_1} is a graph which is not triangle free, then

$$ec_{\mathcal{G}}(v) = 3 \text{ for every vertex } v \in V(\mathcal{G}).$$

Theorem 5 *For $i = 1, 2, 3$, let G_{n_i} be a k_i-regular graph of order n_i and size m_i, where G_{n_1} is triangle-free. Then the Wiener index of $\mathcal{G} = G_{n_1}^C \triangleright (G_{n_2}^V \cup G_{n_3}^E)$ is given by*

$$\begin{aligned} W(\mathcal{G}) = \frac{1}{2}\Big(& n_1^2 - n_1 + 2(n_2^2 + n_3^2 + n_1n_2 - n_2 - n_3 + m_1n_3 + m_1^2) \\ & + 4(n_1n_3 + m_1n_1 + m_1n_2 - m_1) - (n_2k_2 + n_3k_3) + 6n_2n_3\Big). \end{aligned}$$

Proof. Let the vertex set of $\mathcal{G} = G_{n_1}^C \triangleright (G_{n_2}^V \cup G_{n_3}^E)$ be

$$V(\mathcal{G}) = \{v_1, v_2, \dots, v_{n_1}, v_{e_1}, v_{e_2}, \dots, v_{e_{m_1}}, u_1, u_2, \dots, u_{n_2}, w_1, w_2, \dots, w_{n_3}\},$$

where $v_1, v_2, \dots, v_{n_1}$ are the vertices in G_{n_1}, $v_{e_1}, v_{e_2}, \dots, v_{e_{m_1}}$ are the vertices corresponding to the edges of G_{n_1} in $C(G_{n_1})$, $u_1, u_2, \dots, u_{n_2}$ are the vertices in G_{n_2}, and $w_1, w_2, \dots, w_{n_3}$ are the vertices in G_{n_3}. Then

$$\begin{aligned} Tr(v_i) &= n_1 + n_2 + 2n_3 + 2m_1 - 1,\ i = 1, \dots, n_1; \\ Tr(v_{e_j}) &= 2n_1 + 2n_2 + n_3 + 2m_1 - 4,\ j = 1, \dots, m_1; \\ Tr(u_k) &= n_1 + 2n_2 + 3n_3 + 2m_1 - k_2 - 2,\ k = 1, \dots, n_2; \\ Tr(w_l) &= 2n_1 + 3n_2 + 2n_3 + m_1 - k_3 - 2,\ l = 1, \dots, n_3. \end{aligned}$$

From (8),

$$\begin{aligned} W(\mathcal{G}) &= \frac{1}{2} \sum_{v_i \in V(\mathcal{G})} Tr(v_i) \\ &= \frac{1}{2}(n_1^2 - n_1 + 2(n_2^2 + n_3^2 + n_1n_2 - n_2 - n_3 + m_1n_3 + m_1^2) \\ &\quad + 4(n_1n_3 + m_1n_1 + m_1n_2 - m_1) - (n_2k_2 + n_3k_3) + 6n_2n_3). \end{aligned}$$

□

For $i = 1, 2, 3$, let G_{n_i} be a k_i-regular graph of order n_i and size m_i, where G_{n_1} is triangle-free. Then, by using Theorems 3,4 and 5, we get bounds for the spectral radius and energy of $D(\mathcal{G})$.

Corollary 1 *For $\mathcal{G} = G^C_{n_1} \triangleright (G^V_{n_2} \cup G^E_{n_3})$ one has*

$$\mu_1(\mathcal{G}) \geq \frac{1}{n_1+n_2+n_3+m_1}\Big(n_1^2 - n_1 + 2(n_2^2 + n_3^2 + n_1n_2 - n_2 - n_3 + m_1n_3 \\ + m_1^2) + 4(n_1n_3 + m_1n_1 + m_1n_2 - m_1) - (n_2k_2 + n_3k_3) + 6n_2n_3\Big).$$

and

$$E_D(\mathcal{G}) \leq (2-\sqrt{2})\sqrt{n_1+n_2+n_3+m_1}\left(3\sqrt{2} + \frac{1}{2}(n_1^2 - n_1 + 2(n_2^2 + n_3^2 \right. \\ +n_1n_2 - n_2 - n_3 + m_1n_3 + m_1^2) + 4(n_1n_3 + m_1n_1 + m_1n_2 - m_1) \\ \left. -(n_2k_2 + n_3k_3) + 6n_2n_3)\right).$$

Theorem 6 *For $i = 1, 2, 3$, let G_{n_i} be a graph of order n_i and size m_i. Then (i) if G_{n_1} is triangle-free,*

$$\xi^c(\mathcal{G}) = 2n_1^2 + 5n_1n_2 + 5m_1n_3 - 2n_1 + 4m_1 + 6m_2 + 6m_3$$

otherwise,

$$\xi^c(\mathcal{G}) = 3n_1^2 + 6n_1n_2 + 6m_1n_3 - 3n_1 + 6(m_1 + m_2 + m_3);$$

(ii) if G_{n_1} is triangle-free

$$\xi^{ce}(\mathcal{G}) = \frac{1}{6}\Big(3n_1^2 + 5(n_1n_2 + m_1n_3) + 6m_1 + 4(m_2 + m_3) - 3n_1\Big)$$

otherwise,

$$\xi^{ce}(\mathcal{G}) = \frac{1}{3}\Big(n_1^2 + 2(n_1n_2 + m_1n_3) - n_1 + 2(m_1 + m_2 + m_3)\Big).$$

Proof. Let G_{n_1} be a triangle-free graph. From (1) by using (9) and (10), we can write

$$\xi^c(\mathcal{G}) = \sum_{v\in V(G_{n_1})} 2(n_1 + n_2 - 1) + \sum_{v\in I(G_{n_1})} 2(n_3 + 2) \\ + \sum_{v\in V(G_{n_2})} 3(deg_{G_{n_2}}(v) + n_1) + \sum_{v\in V(G_{n_3})} 3(deg_{G_{n_3}}(v) + m_1) \\ = 2n_1^2 + 5n_1n_2 + 5m_1n_3 - 2n_1 + 4m_1 + 6m_2 + 6m_3.$$

Similarly, in the case when G_{n_1} is not a triangle-free graph, by using (9) and (10), we get

$$\xi^c(\mathcal{G}) = 3n_1^2 + 6n_1n_2 + 6m_1n_3 - 3n_1 + 6(m_1 + m_2 + m_3).$$

Let G_{n_1} be a triangle-free graph. Then from (2) using (9) and (10), we obtain

$$\begin{aligned}\xi^{ce}(\mathcal{G}) &= \sum_{v\in V(G_{n_1})} \frac{n_1+n_2-1}{2} + \sum_{v\in I(G_{n_1})} \frac{n_3+2}{2} + \sum_{v\in V(G_{n_2})} \frac{deg_{G_{n_2}}+n_1}{3} \\ &\quad + \sum_{v\in V(G_{n_3})} \frac{deg_{G_{n_3}}+m_1}{3} \\ &= \frac{1}{6}(3n_1^2 + 5(n_1n_2 + m_1n_3) + 6m_1 + 4(m_2+m_3) - 3n_1).\end{aligned}$$

Similarly, in the case when G_{n_1} is not a triangle-free graph, by using (9) and (10), we get

$$\xi^{ce}(\mathcal{G}) = \frac{1}{3}\left(n_1^2 + 2(n_1n_2 + m_1n_3) - n_1 + 2(m_1+m_2+m_3)\right).$$

□

Theorem 7 *For $i = 1, 2, 3$, let G_{n_i} be a graph of order n_i and size m_i. Then*
(i) if G_{n_1} is triangle-free,

$$\tau(\mathcal{G}) = 2n_1 + 2m_1 + 3n_2 + 3n_3,$$

otherwise,

$$\tau(\mathcal{G}) = 3(n_1 + n_2 + n_3 + m_1);$$

(ii) if G_{n_1} is triangle-free,

$$aveg(\mathcal{G}) = \frac{2n_1 + 2m_1 + 3n_2 + 3n_3}{n_1 + n_2 + n_3 + m_1},$$

otherwise, $aveg(\mathcal{G}) = 3$.

Proof. Let G_{n_1} be triangle-free. Then from (3) by using (10), we get

$$\tau(\mathcal{G}) = 2n_1 + 2m_1 + 3n_2 + 3n_3.$$

Similarly, when G_{n_1} is not a triangle-free graph, we obtain

$$\tau(\mathcal{G}) = 3(n_1 + n_2 + n_3 + m_1).$$

From (4), we get

$$aveg(\mathcal{G}) = \frac{\tau(\mathcal{G})}{n_1 + n_2 + n_3 + m_1},$$

and statement (ii) follows. □

Theorem 8 *For $i = 1, 2, 3$, let G_{n_i} be a graph of order n_i and size m_i. Then (i) if G_{n_1} is triangle-free,*

$$M_1(\mathcal{G}) = 4n_1 + 4m_1 + 9n_2 + 9n_3,$$

otherwise,

$$M_1(\mathcal{G}) = 9(n_1 + n_2 + n_3 + m_1);$$

(ii) if G_{n_1} is triangle-free,

$$M_2(\mathcal{G}) = 4m_1 + 9(m_2 + m_3) + 2(n_1^2 - n_1) + 6(n_1n_2 + m_1n_3),$$

otherwise,

$$M_2(\mathcal{G}) = 9(m_1 + m_2 + m_3 + n_1n_2 + m_1n_3 + \frac{n_1^2 - n_1}{2}.$$

Proof. Let G_{n_1} be triangle-free. Then from (5) by using (10), we get

$$\begin{aligned} M_1(\mathcal{G}) &= \sum_{v\in V(G_{n_1})} 2^2 + \sum_{v\in I(G_{n_1})} 2^2 + \sum_{v\in V(G_{n_2})} 3^2 + \sum_{v\in V(G_{n_3})} 3^2 \\ &= 4n_1 + 4m_1 + 9n_2 + 9n_3. \end{aligned}$$

Similarly, when G_{n_1} is not a triangle-free graph, we get

$$M_1(\mathcal{G}) = 9(n_1 + n_2 + n_3 + m_1).$$

Let G_{n_1} be a triangle-free graph. Then from (5) by using (10), we get

$$\begin{aligned} M_2(\mathcal{G}) = &\sum_{uv\in E(G_{n_2})} 3\times 3 + \sum_{uv\in E(G_{n_3})} 3\times 3 + \sum_{\substack{u\in V(G_{n_1}),\\ v\in V(G_{n_2})}} 2\times 3 \\ &+ \sum_{\substack{u\in I(G_{n_1}),\\ v\in V(G_{n_3})}} 2\times 3 + \sum_{\substack{uv\in E(\mathcal{G}),\\ u\in V(G_{n_1}), v\in I(G_{n_1})}} 2\times 2 + \sum_{\substack{uv\in E(\mathcal{G}),\\ u,v\in V(G_{n_1})}} 2\times 2 \\ = &\, 4m_1 + 9m_2 + 9m_3 + 2n_1^2 - 2n_1 + 6n_1n_2 + 6m_1n_3. \end{aligned}$$

Similarly, when G_{n_1} is not a triangle-free graph, we get

$$M_2(\mathcal{G}) = 9\left(m_1 + m_2 + m_3 + n_1n_2 + m_1n_3 + \frac{n_1^2 - n_1}{2}\right).$$

□

Theorem 9 *For $i = 1, 2, 3$, let G_{n_i} be a graph of order n_i and size m_i. Then (i) if G_{n_1} is triangle-free,*

$$GA_4(\mathcal{G}) = \frac{2\sqrt{6}}{5}(n_1n_2 + m_1n_3) + m_1 + m_2 + m_3 + \frac{1}{2}(n_1^2 - n_1),$$

otherwise,

$$GA_4(\mathcal{G}) = m_1 + m_2 + m_3 + n_1n_2 + m_1n_3 + \frac{1}{2}(n_1^2 - n_1).$$

(ii) if G_{n_1} is triangle-free,

$$ABC_5(\mathcal{G}) = \frac{1}{\sqrt{2}}(n_1n_2 + m_1n_3 + m_1) + \frac{2}{3}(m_2 + m_3) + \frac{1}{2\sqrt{2}}(n_1^2 - n_1),$$

otherwise,

$$ABC_5(\mathcal{G}) = \frac{2}{3}(m_1 + m_2 + m_3 + n_1n_2 + m_1n_3) + \frac{1}{3}(n_1^2 - n_1).$$

Proof. Let $\mathcal{G} = G_{n_1}^C \triangleright (G_{n_2}^V \cup G_{n_3}^E)$, where G_{n_1} is triangle-free, then from (6) by using (10) we have

$$\begin{aligned} GA_4(\mathcal{G}) = & \sum_{uv\in E(G_{n_2})} 2\frac{\sqrt{3\times 3}}{3+3} + \sum_{uv\in E(G_{n_3})} 2\frac{\sqrt{3\times 3}}{3+3} + \sum_{\substack{u\in V(G_{n_1}),\\ v\in V(G_{n_2})}} 2\frac{\sqrt{2\times 3}}{2+3} \\ & + \sum_{\substack{u\in I(G_{n_1}),\\ v\in V(G_{n_3})}} 2\frac{\sqrt{2\times 3}}{2+3} + \sum_{\substack{u\in V(G_{n_1}),\\ v\in I(G_{n_1}),\\ uv\in E(\mathcal{G})}} 2\frac{\sqrt{2\times 2}}{2+2} + \sum_{\substack{uv\in E(\mathcal{G}),\\ u,v\in V(G_{n_1})}} 2\frac{\sqrt{2\times 2}}{2+2} \\ & = m_1 + m_2 + m_3 + \frac{2\sqrt{6}}{5}(n_1n_2 + m_1n_3) + \frac{n_1^2 - n_1}{2}. \end{aligned}$$

Similarly, when G_{n_1} is not a triangle-free graph, we get

$$GA_4(\mathcal{G}) = m_1 + m_2 + m_3 + n_1n_2 + m_1n_3 + \frac{n_1^2 - n_1}{2}.$$

Let G_{n_1} be a triangle-free graph. Then from (7) by using (10), we get

$$\begin{aligned} ABC_5(\mathcal{G}) = & \sum_{uv\in E(G_{n_2})} \sqrt{\frac{3+3-2}{3\times 3}} + \sum_{uv\in E(G_{n_3})} \sqrt{\frac{3+3-2}{3\times 3}} \\ & + \sum_{\substack{u\in V(G_{n_1}),\\ v\in V(G_{n_2})}} \sqrt{\frac{2+3-2}{2\times 3}} + \sum_{\substack{u\in I(G_{n_1}),\\ v\in V(G_{n_3})}} \sqrt{\frac{2+3-2}{2\times 3}} \\ & + \sum_{\substack{uv\in E(\mathcal{G}),\\ u\in V(G_{n_1}),\\ v\in I(G_{n_1})}} \sqrt{\frac{2+2-2}{2\times 2}} + \sum_{\substack{uv\in E(\mathcal{G}),\\ u,v\in V(G_{n_1})}} \sqrt{\frac{2+2-2}{2\times 2}} \\ & = \frac{2}{3}(m_2 + m_3) + \frac{1}{\sqrt{2}}\left(n_1n_2 + m_1n_3 + m_1 + \frac{n_1(n_1-1)}{2}\right). \end{aligned}$$

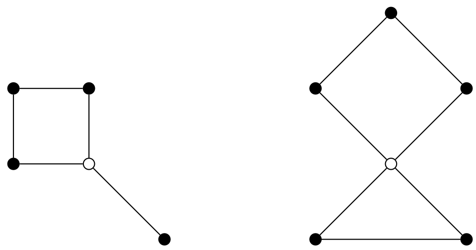

Figure 2: $K_2^C \triangleright (K_1^V \cup K_1^E), K_2^C \triangleright (K_1^V \cup K_2^E)$.

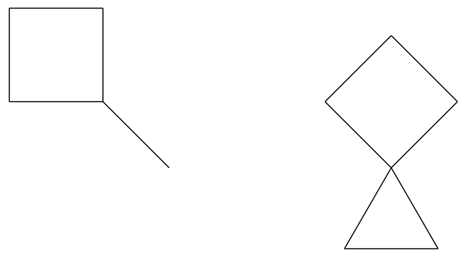

Figure 3: Methylcyclobutane (C_5H_{10}), Spirohexane (C_6H_{10}).

Similarly, when G_{n_1} is not a triangle-free graph, we get

$$ABC_5(\mathcal{G}) = \frac{2}{3}(m_1 + m_2 + m_3 + n_1n_2 + m_1n_3) + \frac{n_1(n_1-1)}{3}.$$

□

Example The molecular graph of Methylcyclobutane (C_5H_{10}) is isomorphic to $K_2^C \triangleright (K_1^V \cup K_1^E)$, and that of Spirohexane (C_6H_{10}) is isomorphic to $K_2^C \triangleright (K_1^V \cup K_2^E)$ as shown in Fig. 2 and 3. Then the following table gives different topological indices of the molecules Methylcyclobutane and Spirohexane.

No.	Topological indices	Methylcyclobutane (C_5H_{10})	Spirohexane (C_6H_{10})
1	Wiener index	16	25
2	Eccentric connectivity index	23	18
3	Connective eccentricity index	4.5	6
4	Total-eccentricity index	12	15
5	Average eccentricity	3	2.5
6	First Zagreb index	30	39
7	Second Zagreb index	26	41
8	Geometric-arithmetic index	4.939	6.919
9	Atom-bond connectivity index	3.535	4.909

3 Conclusion

Topological indices play an important role in mathematical chemistry. In QSAR/QSPR study, topological indices can be used to estimate the bioactivity of chemical compounds. In modelling the chemical and other properties of molecules, we can use topological indices as a tool. This article gives the results related to various topological indices of the newly defined graph operation called central vertex-edge join (CVE-join). From these results, we compute different topological indices of the chemical compounds Methylcyclobutane (C_5H_{10}) and Spirohexane (C_6H_{10}). Also, the D-spectrum of CVE-join of three regular graphs G_{n_1}, G_{n_2} and G_{n_3} when G_{n_1} is a triangle-free are obtained. These results enable us to construct new D-equienergetic graph families. In addition, bounds for the distance spectral radius and distance energy of CVE-join of three graphs are calculated.

Acknowledgements. The authors would like to thank the DST, Government of India, for providing support to carry out this work under the scheme 'FIST'(No.SR/FST/MS-I/2019/40).

References

[1] G. Aalipour, A. Abiad, Z. Berikkyzy, J. Cummings, D.S. Jessica, W. Gao, K. Heysse, L. Hogben, F.H.J. Kenter, M. Tait, and J.C.H. Lin, On the distance spectra of graphs. Linear Algebra Appl., **497** (2016), pp. 66–87. https://doi.org/10.1016/j.laa.2016.02.018

[2] M. Aouchiche and P. Hansen, Distance spectra of graphs: A survey. Linear Algebra Appl., **458** (2014), pp. 301–386. https://doi.org/10.1016/j.laa.2014.06.010

[3] A.E. Brouwer and W.H. Haemers, *Spectra of graphs*, Springer: New York, USA, 2012.

[4] F. Buckley and F. Harary, *Distance in graphs*, **2**, Addison-Wesley Redwood City, CA, 1990.

[5] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of graphs: Theory and applications*, 3rd edition, Johann Ambrosius Barth Verlag, Heidelberg, Leipzig, 1995. https://doi.org/10.1017/s0013091500022902

[6] K.C. Das and I. Gutman, Upper bounds on distance energy. MATCH Commun. Math. Comput. Chem., **86** (2021), pp.611–620.

[7] M.R. Farahani, Eccentricity version of atom-bond connectivity index of benzenoid family $ABC_5(H_k)$. World Appl. Sci. J. Chem., **21** (2013), no. 9, pp. 1260–1265.

[8] M. Ghorbani, Connective eccentric index of fullerenes. J. Math. Nanosci., **1** (2011), pp. 43–50.

[9] M. Ghorbani and M.A. Hosseinzadeh, A new version of Zagreb indices. Filomat, **26** (2012), no. 1, pp. 93–100. https://doi.org/10.2298/fil1201093g

[10] M. Ghorbani and A. Khaki, A note on the fourth version of geometric-arithmetic index. Optoelectron. Adv. Mat., **4** (2010), no. 12, pp. 2212–2215.

[11] S. Gupta, M. Singh and A.K. Madan, Connective eccentricity index: A novel topological descriptor for predicting biological activity. J. Mol. Graph. Model., **18** (2000), no. 1, pp. 18–25. https://doi.org/10.1016/s1093-3263(00)00027-9

[12] T. Haritha, and A.V. Chithra, On the distance spectra of central vertex join and central edge join of two regular graphs. Ricerche di Matematica, 2022, 19 pp. https://doi.org/10.1007/s11587-022-00721-5

[13] A. Ilić, Distance spectra and distance energy of integral circulant graphs. Linear Algebra Appl., **433** (2010), no. 5, pp. 1005–1014. https://doi.org/10.1016/j.laa.2010.04.034

[14] G. Indulal, C.S. Deena and X. Liuc, The distance spectrum of the subdivision vertex join and subdivision edge join of two regular graphs. Discrete Math. Lett., **1** (2019), pp. 36–41.

[15] G. Indulal, I. Gutman and A. Vijayakumar, On distance energy of graphs. MATCH Commun. Math. Comput. Chem., **60** (2008), no. 2, pp. 461–472.

[16] T.K. Jahfar and A.V. Chithra, Central vertex join and central edge join of two graphs. AIMS Mathematics, **5** (2020), no. 6, pp. 7214–7233. https://doi.org/10.3934/math.2020461

[17] H.S. Ramane, I. Gutman and D.S. Revankar, Distance equienergetic graphs. MATCH Commun. Math. Comput. Chem., **60** (2008), pp. 473–484.

[18] V. Sharma, R. Goswami and A.K. Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies. J. Chem. Inf. Comput. Sci., **37** (1997), no. 2, pp. 273–282. https://doi.org/10.1021/ci960049h

[19] V.A. Skorobogatov and A.A. Dobrynin, Metric analysis of graphs. MATCH Commun. Math. Comput. Chem., **23** (1988), no. 1, pp. 105–151.

[20] J.V. Vivin, M.M. Akbar Ali and K. Thilagavathi, On harmonious coloring of central graphs. Advances and Applications in Discrete Mathematics, **2** (2008), no. 1, pp. 17–33.

[21] H. Wiener, Structural determination of paraffin boiling points. J. Am. Chem. Soc., **69** (1947), no. 1, pp. 17–20. https://doi.org/10.1021/ja01193a005

[22] B. Zhou and N. Trinajstić, On the largest eigenvalue of the distance matrix of a connected graph. Chem. Phys. Lett., **447** (2007), no. 4-6, pp. 384–387. https://doi.org/10.1016/j.cplett.2007.09.048

Haritha Thottungal
Department of Mathematics,
National Institute of Technology Calicut,
Calicut-673 601, Kerala, India.
harithathottungal96@gmail.com

Chithra A. Velu
Department of Mathematics,
National Institute of Technology Calicut,
Calicut-673 601, Kerala, India.
chithra@nitc.ac.in

Please, cite to this paper as published in
Armen. J. Math., V. **15**, N. 10(2023), pp. 1–16
https://doi.org/10.52737/18291163-2023.15.10-1-16