NANOSYSTEMS:
PHYSICS, CHEMISTRY, MATHEMATICS

Original article

Shashwath S. Shetty, et al. *Nanosystems: Phys. Chem. Math.*, 2024, **15** (3), 315–324.
http://nanojournal.ifmo.ru
DOI 10.17586/2220-8054-2024-15-3-315-324

Energy and spectral radius of Zagreb matrix of graph with applications

Shashwath S. Shetty[1,a], K. Arathi Bhat[1,b]

[1]Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India

[a]shashwathsshetty01334@gmail.com, [b]arathi.bhat@manipal.edu

Corresponding author: K. Arathi Bhat, arathi.bhat@manipal.edu

ABSTRACT The $\mathcal{Z}$-matrix of a simple graph Γ is a square symmetric matrix, whose rows and columns correspond to the vertices of the graph and the ij^{th} entry is equal to the sum of the degrees of i^{th} and j^{th} vertex, if the corresponding vertices are adjacent in Γ, and zero otherwise. The Zagreb eigenvalues of Γ are the eigenvalues of its $\mathcal{Z}$-matrix and the Zagreb energy of Γ is the sum of absolute values of its Zagreb eigenvalues. We study the change in Zagreb energy of a graph when the edges of the graph are deleted or rotated. Suppose Γ is a graph obtained by identifying $u \in \mathcal{V}(\Gamma_1)$ and $v \in \mathcal{V}(\Gamma_2)$ or adding an edge between u and v, then it is important to study the relation between Zagreb energies of Γ_1, Γ_2 and Γ. The highlight of the paper is that, the acentric factor of n-alkanes appear to have a strong positive correlation (where the correlation coefficient is 0.9989) with energy of the $\mathcal{Z}$-matrix. Also, the novel correlation of the density and refractive index of n-alkanes with spectral radius of the $\mathcal{Z}$-matrix has been observed.

KEYWORDS spectral radius, energy, Zagreb matrix, acentric factor, density, refractive index

ACKNOWLEDGEMENTS We acknowledge the Institution for overall support. The authors sincerely appreciate the reviewers for all the valuable comments and suggestions, which helped to improve the quality of the manuscript.

FOR CITATION Shashwath S. Shetty, K. Arathi Bhat Energy and spectral radius of Zagreb matrix of graph with applications. *Nanosystems: Phys. Chem. Math.*, 2024, **15** (3), 315–324.

1. Introduction

In mathematical chemistry, graph energies have received considerable attention because of their immense applications [1].Recently, various types of matrices and the corresponding energies of graphs have been studied. In 1978, Gutman defined the energy [2] of a simple graph as the sum of the absolute values of eigenvalues of the adjacency matrix of the corresponding graph.

Let $\Gamma = (\mathcal{V}, E)$ be an undirected graph on a finite non-empty set of vertices $\mathcal{V}$ and the prescribed collection E of an unordered pair of vertices called edges. Two vertices are said to be adjacent, if they share an edge. We use $i \sim j$ to denote that vertices i and j are adjacent. The neighborhood of vertex i in graph Γ is a collection of all vertices that are adjacent to i in Γ. The adjacency matrix of a graph Γ denoted by $\mathcal{A}^\Gamma$ is $n \times n$ matrix whose rows and columns correspond to the vertices of the graphs and the ij^{th} entry is one if vertex i is adjacent to vertex j, and zero otherwise. The energy of a graph is defined as the sum of absolute values of eigenvalues of adjacency matrix of the graph. The singular values of a real matrix $\mathcal{A}$ is the square root of the eigenvalues of $\mathcal{A}^\intercal\mathcal{A}$, where $\mathcal{A}^\intercal$ is the transpose of the matrix $\mathcal{A}$. For a real symmetric positive definite matrix, the singular values of the matrix coincide with the eigenvalues of the matrix. Let $\mathcal{A}^\Gamma_{TI}$ is an extended adjacency matrix of the graph Γ corresponding to the degree based symmetric topological index TI, and $\mathcal{A}^\Gamma_{TI}[u]$ be a matrix obtained from $\mathcal{A}^\Gamma_{TI}$ by deleting the row and column corresponding to the vertex u, where u is a vertex of the graph Γ.

The first extended adjacency matrix corresponding to a degree based topological index defined was the Randić matrix [3], and the energy of the corresponding matrix was defined in a similar manner and termed as the Randić energy. The first Zagreb index, $M_1(\Gamma)$ of a graph Γ is defined [4] as the sum of the squares of the degrees over all vertices of the graph. Interesting facts concerned with the first Zagreb index are available in the literature [5, 6] and recently it has been considered for graphs with self-loops [7].

The first Zagreb matrix ($\mathcal{Z}$-matrix) [8] of a graph Γ denoted by $\mathcal{Z}^\Gamma$ is an $n \times n$ matrix whose rows and columns correspond to the vertices of the graph and it's ij^{th} entry, z_{ij} is given by

$$z_{ij} = \begin{cases} d_i + d_j, & \text{if } i \sim j; \\ 0, & \text{otherwise,} \end{cases}$$

where d_i is the degree of vertex $i \in \mathcal{V}(\Gamma)$. The Zagreb energy of a simple graph Γ is defined as the sum of the absolute values of the Zagreb matrix eigenvalues of the graph. Let $\zeta_1 \geq \zeta_2 \geq \cdots \geq \zeta_n$ be the eigenvalues and ζ_1 be the $\mathcal{Z}$-spectral radius corresponding to the $\mathcal{Z}$-matrix of the graph Γ. If x is the principal eigenvector of the $\mathcal{Z}$-matrix then the Rayleigh

quotient of $\mathcal{Z}$ is a scalar, $\frac{x^\intercal \mathcal{Z} x}{x^\intercal x}$ and, the supremum value of this quotient over all the vectors x gives one the spectral radius of $\mathcal{Z}$, i.e.,

$$\zeta_1 = \sup_x \frac{x^\intercal \mathcal{Z} x}{x^\intercal x}.$$

For all other undefined terminologies of graph theory reader can refer [9].

A few bounds for $\mathcal{Z}$-spectral radius and its variation during deletion and the rotation of an edge is discussed in Section 2. In Section 3, the relation between Zagreb energies of Γ_1, Γ_2 and Γ is discussed, where Γ is a graph obtained by identifying $u \in \mathcal{V}(\Gamma_1)$ and $v \in \mathcal{V}(\Gamma_2)$ or adding an edge between u and v. Chemical applications of $\mathcal{Z}$-spectral radius and Zagreb energy is discussed in the last section.

2. $\mathcal{Z}$-spectral Radius

An edge rotation of $e = xy \in E(\Gamma)$ around $x \in \mathcal{V}(\Gamma)$, replaces xy by an edge xw where $xw \notin E(\Gamma)$. The variation of $\mathcal{Z}$-spectral radius during the deletion and rotation of an edge is discussed in this section along with few bounds.

Theorem 1. *Let Γ be a connected graph of order n, maximum degree Δ and $\mathcal{Z}$-spectral radius ζ_1. If $M_1(\Gamma)$ denotes the first Zagreb index of the graph Γ, then*

$$\frac{M_1(\Gamma) + \sum\limits_{u \in \mathcal{V}} d_{2,u}}{n} \leq \zeta_1 \leq 2\Delta^2,$$

where $d_{2,u}$ is is the sum of degrees of all the vertices which are adjacent to u in Γ. Equality holds in both if and only if Γ is regular.

Proof. Now,

$$\zeta_1 \geq \frac{J^\intercal \mathcal{Z} J}{J^\intercal J} = \frac{\sum\limits_{u \in \mathcal{V}(\Gamma)} (d_u^2 + d_{2,u})}{n} = \frac{M_1(\Gamma) + \sum\limits_{u \in \mathcal{V}(\Gamma)} d_{2,u}}{n},$$

where $d_{2,u}$ is is the sum of degrees of all the vertices which are adjacent to u in Γ. Since, the all one vector $\mathbf{J}$ is the eigenvector corresponding to the regular graph Γ, equality holds in the above if and only if Γ is a regular graph.
Let x_u is the maximum component of the principal eigenvector x. The eigenvalue equation for the $\mathcal{Z}$-matrix of the simple graph is given by,

$$\zeta_1 x_u = \sum_{v \in N(u)} (d_u + d_v) x_v.$$

Therefore,

$$\begin{aligned} \zeta_1 x_u = \sum_{v \in N(u)} (d_u + d_v) x_v &\leq \sum_{v \in N(u)} (d_u + d_v) x_u \\ &\leq 2\Delta \sum_{v \in N(u)} x_u \\ &\leq 2\Delta^2 x_u. \end{aligned}$$

Equality holds in the above if and only if $d_u = d_v = \Delta$, i.e., Γ is regular. □

Theorem 2. *[10] Suppose that $\mathcal{A} = (a_{ij})$ and $\mathcal{B} = (b_{ij})$ are two $n \times n$ non-negative symmetric matrices. If $\mathcal{A} \leq \mathcal{B}$, i.e., $a_{ij} \leq b_{ij}$ for all i, j, then $\zeta_1(A) \leq \zeta_1(B)$. Furthermore, if B is irreducible and $\mathcal{A} \neq \mathcal{B}$, then $\zeta_1(A) < \zeta_1(B)$.*

Theorem 3. *Let Γ be a forest of order n and size m with $n \leq 2m$. Then*

$$2 \leq \zeta_1(\Gamma) \leq n\sqrt{2m - n + 1},$$

with equality in the lower bound holds if and only if $\Gamma \cong \frac{n}{2} K_2$ and equality in the upper bound holds if and only if Γ isomorphic to the star S_n.
Furthermore for $n > 2$, if Γ is connected, then

$$6 \cos \frac{\pi}{n+1} \leq \zeta_1(P_n) \leq \zeta_1(\Gamma)$$

with equality if and only if $\Gamma \cong P_3$

Proof. Since Γ is a forest, we have $d_i + d_j \leq n$ for every i, j in $\mathcal{V}(\Gamma)$. Hence,

$$\mathcal{Z}^\Gamma \leq n\mathcal{A}^\Gamma, \tag{1}$$

where $\mathcal{A}^\Gamma$ is the adjacency matrix of the graph Γ. Here, the equality in (1) holds if and only if Γ is a star graph. Now by using Theorem 2 , $\zeta_1 \leq n\rho$, where ρ is the adjacency spectral radius of the graph. But, we have [11] $\rho \leq \sqrt{2m - n + 1}$ and the equality follows if and only if the graph is a star graph or a complete graph on n vertices.

As $n \leq 2m$, we have

$$2\mathcal{A}^{\Gamma} \leq \mathcal{Z}^{\Gamma}$$

with equality if and only if $\Gamma \cong \frac{n}{2}K_2$.
Furthermore, when Γ is connected and $n \geq 3$, we have

$$3\mathcal{A}^{\Gamma} \leq \mathcal{Z}^{\Gamma}$$

with equality if and only if Γ is a path graph on 3 vertices. We know that,

$$\rho(P_n) = 2\cos\frac{\pi}{n+1},$$

from which the result follows. □

Theorem 4. *Let Γ be a connected graph with the $\mathcal{Z}$-spectral radius ζ_1 and the corresponding principal eigenvector x. If $e = uv$ is not an edge in Γ, then*

$$\zeta_1(\Gamma + e) > \zeta_1(\Gamma).$$

Proof. Let x_u denote the u^{th} component of the eigenvector x, corresponding to the spectral radius of Γ. By using Rayleigh quotient

$$\zeta_1(\Gamma + e) \geq \frac{x^{\intercal}\mathcal{Z}^{\Gamma+e}x}{x^{\intercal}x} = \frac{x^{\intercal}\mathcal{Z}^{\Gamma}x}{x^{\intercal}x} + \frac{x^{\intercal}\mathcal{C}_1 x}{x^{\intercal}x},$$

where

$$\mathcal{C}_1 = \begin{bmatrix} \mathbf{0}_{n-2\times n-2} & \mathbf{J}_u & \mathbf{J}_v \\ \mathbf{J}_u^{\intercal} & \mathbf{0} & d_u + d_v + 2 \\ \mathbf{J}_v^{\intercal} & d_u + d_v + 2 & \mathbf{0} \end{bmatrix},$$

and d_u and d_v are the degrees of the vertices u and v respectively, in the graph Γ. $\mathbf{J}_u$ is the column vector of size $(n-2)$ corresponding to the vertex u, whose entries are 0 or 1, accordingly the corresponding vertex is adjacent to u or not. Similarly, the column vector $\mathbf{J}_v$ corresponds to the vertex v. Therefore

$$\frac{x^{\intercal}\mathcal{C}_1 x}{x^{\intercal}x} = \frac{M}{x^{\intercal}x},$$

where $M = 2(d_u + d_v + 2)x_u x_v + 2\sum_{w\sim u} x_u x_w + 2\sum_{y\sim v} x_v x_y$.
Here M is strictly greater than zero, since x is a positive eigenvector [12]. □

Theorem 5. *Let p, q, r be the vertices of a connected graph Γ such that rp is an edge in Γ, where as rq is not an edge in Γ. Then*

$$\zeta_1(\Gamma - rp + rq) \geq \zeta_1(\Gamma), \text{ if } N \geq 0$$

and the inequality is strict if $N > 0$,
where $N = d_r(x_q - x_p)x_r + (d_q x_q + x_q - d_p x_p)x_r + \sum_{y\sim q, y\neq r} x_q x_y - \sum_{w\sim p, w\neq r} x_p x_w$.

Proof. Let x be the eigenvector corresponding to $\zeta_1(\Gamma)$. Then, we have

$$\zeta_1(\Gamma - rp + rq) \geq \frac{x^{\intercal}\mathcal{Z}^{(\Gamma-rp+rq)}x}{x^{\intercal}x} = \frac{x^{\intercal}\mathcal{Z}^{\Gamma}x}{x^{\intercal}x} + \frac{x^{\intercal}\mathcal{C}_2 x}{x^{\intercal}x},$$

where

$$\mathcal{C}_2 = \begin{bmatrix} \mathbf{0}_{n-3\times n-3} & \mathbf{0}_{n-3\times 1} & -\mathbf{J}_p & \mathbf{J}_q \\ \mathbf{0}_{1\times n-3} & \mathbf{0} & -(d_r + d_p) & d_r + d_q + 1 \\ -\mathbf{J}_p^{\intercal} & -(d_r + d_p) & \mathbf{0} & \mathbf{0} \\ \mathbf{J}_q^{\intercal} & d_r + d_q + 1 & \mathbf{0} & \mathbf{0} \end{bmatrix},$$

where d_p, d_q and d_r are the degrees of the vertices p, q and r respectively, in the graph Γ. $\mathbf{J}_p$ is the column vector of size $(n-3)$ corresponding to the vertex p, whose entries are 0 or 1, accordingly the corresponding vertex is adjacent to p or not. Similarly, the column vector $\mathbf{J}_q$ corresponds to the vertex q. Hence

$$\frac{x^{\intercal}\mathcal{C}_2 x}{x^{\intercal}x} = \frac{2N}{x^{\intercal}x},$$

where $2N = 2(d_r + d_q + 1)x_r x_q - 2(d_r + d_p)x_r x_p + 2\sum_{y\sim q, y\neq r} x_q x_y - 2\sum_{w\sim p, w\neq r} x_p x_w$. □

3. Zagreb energy

The coalescence of two graphs Γ_1 and Γ_2 denoted by $\Gamma_1 \circ \Gamma_2$ is obtained by identifying two arbitrary vertices, $u \in \mathcal{V}(\Gamma_1)$ and $v \in \mathcal{V}(\Gamma_2)$. The change in adjacency energy during the coalescence of two graphs was studied in [13]. Similar type result is discussed below for the Zagreb energy.

Theorem 6. *Let $\Gamma_1 \circ \Gamma_2$ be coalescence of two graphs Γ_1 and Γ_2 obtained by identifying the vertices $u \in \mathcal{V}(\Gamma_1)$ and $v \in \mathcal{V}(\Gamma_2)$. Then*

$$\mathcal{ZE}(\Gamma_1 \circ \Gamma_2) \leq \mathcal{ZE}(\Gamma_1) + \mathcal{ZE}(\Gamma_2) + 2d_u\sqrt{d_v} + 2d_v\sqrt{d_u}$$

with equality if and only if u is an isolated vertex in Γ_1 and / or v is an isolated vertex in Γ_2.

Proof. It is direct that

$$\mathcal{Z}^{\Gamma_1\circ\Gamma_2} = \begin{bmatrix} \mathcal{Z}^{\Gamma_1}[u] & [x_1+x_2] & \mathbf{0} \\ [x_1+x_2]^\intercal & \mathbf{0} & [y_1+y_2]^\intercal \\ \mathbf{0} & [y_1+y_2] & \mathcal{Z}^{\Gamma_2}[v] \end{bmatrix},$$

where x_1 is the deleted column of $\mathcal{Z}^{\Gamma_1}$ corresponding to the vertex u and x_2 is the column vector obtained by replacing all the non-zero entries of x_1 by d_v. Similarly, y_2 is the deleted column of $\mathcal{Z}^{\Gamma_2}$ corresponding to the vertex v and y_1 is the column vector obtained by replacing all the non-zero entries of y_2 by d_u. Now,

$$\mathcal{Z}^{\Gamma_1\circ\Gamma_2} = \mathcal{A}_1 + \mathcal{A}_2,$$

where

$$\mathcal{A}_1 = \begin{bmatrix} \mathcal{Z}^{\Gamma_1}[u] & [x_1+x_2] & \mathbf{0} \\ [x_1+x_2]^\intercal & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \text{ and}$$

$$\mathcal{A}_2 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & [y_1+y_2]^\intercal \\ \mathbf{0} & [y_1+y_2] & \mathcal{Z}^{\Gamma_2}[v] \end{bmatrix}.$$

For a symmetric matrix singular values are nothing but the absolute values of the eigenvalues and hence by using the Ky Fan's inequality [13] for singular values of the matrix, we have

$$\mathcal{E}(\mathcal{Z}^{\Gamma_1\circ\Gamma_2}) \leq \mathcal{E}(\mathcal{A}_1) + \mathcal{E}(\mathcal{A}_2) \tag{2}$$

and the equality holds if and only if there exists an orthogonal matrix $\mathcal{Q}$ such that both $\mathcal{QA}_1$ and $\mathcal{QA}_2$ are positive semi-definite. Since $\mathcal{Q}$ is orthogonal,

$$\mathcal{Q}^\intercal\mathcal{Q} = \begin{bmatrix} \mathbf{Q_{11}^\intercal} & \mathbf{Q_{21}^\intercal} & \mathbf{Q_{31}^\intercal} \\ \mathbf{Q_{12}^\intercal} & \mathbf{Q_{22}^\intercal} & \mathbf{Q_{32}^\intercal} \\ \mathbf{Q_{13}^\intercal} & \mathbf{Q_{23}^\intercal} & \mathbf{Q_{33}^\intercal} \end{bmatrix} \begin{bmatrix} \mathbf{Q_{11}} & \mathbf{Q_{12}} & \mathbf{Q_{13}} \\ \mathbf{Q_{21}} & \mathbf{Q_{22}} & \mathbf{Q_{23}} \\ \mathbf{Q_{31}} & \mathbf{Q_{32}} & \mathbf{Q_{33}} \end{bmatrix} = \mathbf{I},$$

where the blocks $\mathbf{Q_{ij}}'s$ are of appropriate size. Therefore

$$\begin{aligned} \mathbf{Q_{11}^\intercal Q_{11}} + \mathbf{Q_{21}^\intercal Q_{21}} + \mathbf{Q_{31}^\intercal Q_{31}} &= \mathbf{I}, \\ \mathbf{Q_{13}^\intercal Q_{13}} + \mathbf{Q_{23}^\intercal Q_{23}} + \mathbf{Q_{33}^\intercal Q_{33}} &= \mathbf{I}, \\ \mathbf{Q_{11}^\intercal Q_{13}} + \mathbf{Q_{21}^\intercal Q_{23}} + \mathbf{Q_{31}^\intercal Q_{33}} &= \mathbf{0}. \end{aligned}$$

Consider,

$$\mathcal{QA}_1 = \begin{bmatrix} \mathbf{Q_{11}}\mathcal{Z}^{\Gamma_1}[u] + \mathbf{Q_{12}}[x_1+x_2]^\intercal & \mathbf{Q_{11}}[x_1+x_2] & \mathbf{0} \\ \mathbf{Q_{21}}\mathcal{Z}^{\Gamma_1}[u] + \mathbf{Q_{22}}[x_1+x_2]^\intercal & \mathbf{Q_{21}}[x_1+x_2] & \mathbf{0} \\ \mathbf{Q_{31}}\mathcal{Z}^{\Gamma_1}[u] + \mathbf{Q_{32}}[x_1+x_2]^\intercal & \mathbf{Q_{31}}[x_1+x_2] & \mathbf{0} \end{bmatrix},$$

which implies $\mathbf{Q_{31}}[x_1+x_2] = 0$. Also,

$$\mathcal{QA}_2 = \begin{bmatrix} \mathbf{0} & \mathbf{Q_{13}}[y_1+y_2] & \mathbf{Q_{12}}[y_1+y_2]^\intercal + \mathbf{Q_{13}}\mathcal{Z}^{\Gamma_2}[v] \\ \mathbf{0} & \mathbf{Q_{23}}[y_1+y_2] & \mathbf{Q_{22}}[y_1+y_2]^\intercal + \mathbf{Q_{23}}\mathcal{Z}^{\Gamma_2}[v] \\ \mathbf{0} & \mathbf{Q_{33}}[y_1+y_2] & \mathbf{Q_{32}}[y_1+y_2]^\intercal + \mathbf{Q_{33}}\mathcal{Z}^{\Gamma_2}[v] \end{bmatrix},$$

which implies $\mathbf{Q_{13}}[y_1 + y_2] = 0$. Hence,

$$[\mathbf{Q_{11}}[x_1 + x_2]]^{\intercal}\mathbf{Q_{13}}[y_1 + y_2] + [\mathbf{Q_{21}}[x_1 + x_2]]^{\intercal}\mathbf{Q_{23}}[y_1 + y_2] + [\mathbf{Q_{31}}[x_1 + x_2]]^{\intercal}\mathbf{Q_{33}}[y_1 + y_2] = \mathbf{0}$$

implies

$$[\mathbf{Q_{21}}[x_1 + x_2]]^{\intercal}\mathbf{Q_{23}}[y_1 + y_2] = 0,$$

and here both $\mathbf{Q_{21}}[x_1 + x_2]$ or $\mathbf{Q_{23}}[y_1 + y_2]$ are scalars.
Now if $\mathbf{Q_{21}}[x_1 + x_2] = 0$, and since $\mathcal{QA}_1$ is diagonally dominant we arrive at $[x_1 + x_2] = 0$, which implies that u is an isolated vertex in Γ_1. Similarly if $\mathbf{Q_{23}}[y_1 + y_2] = 0$, we arrive at $[y_1 + y_2] = 0$, which implies that v is an isolated vertex in Γ_2. Let

$$\mathcal{A}_1 = \mathcal{A}_3 + \mathcal{A}_4 \text{ and } \mathcal{A}_2 = \mathcal{A}_5 + \mathcal{A}_6,$$

where

$$\mathcal{A}_3 = \begin{bmatrix} \mathcal{Z}^{\Gamma_1}[u] & x_1 & \mathbf{0} \\ x_1^{\intercal} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}, \ \mathcal{A}_4 = \begin{bmatrix} \mathbf{0} & x_2 & \mathbf{0} \\ x_2^{\intercal} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix},$$

$$\mathcal{A}_5 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & y_2^{\intercal} \\ \mathbf{0} & y_2 & \mathcal{Z}^{\Gamma_2}[v] \end{bmatrix} \text{ and } \mathcal{A}_6 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & y_1^{\intercal} \\ \mathbf{0} & y_1 & \mathbf{0} \end{bmatrix}.$$

Again by using the same inequality,

$$\begin{aligned} \mathcal{E}(\mathcal{A}_1) &\leq \mathcal{E}(\mathcal{A}_3) + \mathcal{E}(\mathcal{A}_4) \\ &= \mathcal{ZE}(\Gamma_1) + 2\sqrt{x_2^{\intercal}x_2} = \mathcal{ZE}(\Gamma_1) + 2\sqrt{d_u d_v^2} \end{aligned}$$

and the equality holds if and only if either u is an isolated vertex in Γ_1 or v is an isolated vertex in Γ_2.
Similarly,

$$\begin{aligned} \mathcal{E}(\mathcal{A}_2) &\leq \mathcal{E}(\mathcal{A}_5) + \mathcal{E}(\mathcal{A}_6) \\ &= \mathcal{ZE}(\Gamma_2) + 2\sqrt{y_1^{\intercal}y_1} = \mathcal{ZE}(\Gamma_2) + 2\sqrt{d_v d_u^2} \end{aligned}$$

with equality condition as stated above. □

The change in Zagreb energy by adding an edge between the two vertices of two different graphs is given below.

Theorem 7. *Let Γ be a graph obtained by adding a bridge $e = uv$ between the vertices $u \in \mathcal{V}(\Gamma_1)$ and $v \in \mathcal{V}(\Gamma_2)$ and let d'_u and d'_v be the degrees of the vertices u and v in the original graphs Γ_1 and Γ_2 respectively. Then*

$$\mathcal{ZE}(\Gamma) \leq \mathcal{ZE}(\Gamma_1) + \mathcal{ZE}(\Gamma_2) + 2(\sqrt{d'_u} + \sqrt{d'_v} + d'_u + d'_v + 2)$$

and the equality holds if and only if u and v are isolated vertices in Γ.

Proof. The $\mathcal{Z}$-matrix corresponding to the above mentioned graph Γ is,

$$\mathcal{Z}^{\Gamma} = \begin{bmatrix} \mathcal{Z}^{\Gamma_1}[u] & [x_1 + \mathbf{J}_u] & \mathbf{0} & \mathbf{0} \\ [x_1 + \mathbf{J}_u]^{\intercal} & \mathbf{0} & d'_u + d'_v + 2 & \mathbf{0} \\ \mathbf{0} & d'_u + d'_v + 2 & \mathbf{0} & [y_1 + \mathbf{J}_v]^{\intercal} \\ \mathbf{0} & \mathbf{0} & [y_1 + \mathbf{J}_v] & \mathcal{Z}^{\Gamma_2}[v] \end{bmatrix}.$$

Here x_1 (and y_1) represents the column vector of $\mathcal{Z}^{\Gamma_1}$ (and $\mathcal{Z}^{\Gamma_2}$) corresponding to the vertex u (and v) in the respective graph. The column vector $\mathbf{J}_u$ is obtained by replacing all the non-zero entries of x_1 by 1 and, the column vector $\mathbf{J}_v$ is obtained by replacing all the non-zero entries of y_1 by 1.

$$\mathcal{Z}^{\Gamma} = \mathcal{B}_1 + \mathcal{B}_2$$

where

$$\mathcal{B}_1 = \begin{bmatrix} \mathcal{Z}^{\Gamma_1}[u] & x_1 & \mathbf{0} & \mathbf{0} \\ x_1^\intercal & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & y_1^\intercal \\ \mathbf{0} & \mathbf{0} & y_1 & \mathcal{Z}^{\Gamma_2}[v] \end{bmatrix}$$

and

$$\mathcal{B}_2 = \begin{bmatrix} \mathbf{0} & \mathbf{J}_u & \mathbf{0} & \mathbf{0} \\ \mathbf{J}_u^\intercal & \mathbf{0} & d'_u + d'_v + 2 & \mathbf{0} \\ \mathbf{0} & d'_u + d'_v + 2 & \mathbf{0} & \mathbf{J}_v^\intercal \\ \mathbf{0} & \mathbf{0} & \mathbf{J}_v & \mathbf{0} \end{bmatrix}.$$

Hence by using the singular values inequality,

$$\mathcal{Z}\mathcal{E}(\Gamma) \leq \mathcal{E}(\mathcal{B}_1) + \mathcal{E}(\mathcal{B}_2). \tag{3}$$

Now, it is easy to observe that

$$\mathcal{E}(\mathcal{B}_1) = \mathcal{Z}\mathcal{E}(\Gamma_1) + \mathcal{Z}\mathcal{E}(\Gamma_2).$$

Let

$$\mathcal{B}_2 = \mathcal{B}_3 + \mathcal{B}_4,$$

where

$$\mathcal{B}_3 = \begin{bmatrix} \mathbf{0} & \mathbf{J}_u & \mathbf{0} & \mathbf{0} \\ \mathbf{J}_u^\intercal & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{J}_v^\intercal \\ \mathbf{0} & \mathbf{0} & \mathbf{J}_v & \mathbf{0} \end{bmatrix}$$

and

$$\mathcal{B}_4 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & d'_u + d'_v + 2 & \mathbf{0} \\ \mathbf{0} & d'_u + d'_v + 2 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}.$$

Therefore by applying the same inequality again, we get

$$\mathcal{E}(\mathcal{B}_2) \leq \mathcal{E}(\mathcal{B}_3) + \mathcal{E}(\mathcal{B}_4) = 2\sqrt{d'_u} + 2\sqrt{d'_v} + 2(d'_u + d'_v + 2). \tag{4}$$

Equality holds in the inequality (4), if and only if there exists an orthogonal matrix $\mathcal{Q}$, such that both $\mathcal{Q}\mathcal{B}_3$ and $\mathcal{Q}\mathcal{B}_4$ are positive semi-definite. If we assume the existence of such an orthogonal matrix $\mathcal{Q}$, we have

$$\begin{aligned} \mathcal{Q}^\intercal\mathcal{Q} &= \\ &= \begin{bmatrix} \mathbf{Q_{11}^\intercal} & \mathbf{Q_{21}^\intercal} & \mathbf{Q_{31}^\intercal} & \mathbf{Q_{41}^\intercal} \\ \mathbf{Q_{12}^\intercal} & \mathbf{Q_{22}^\intercal} & \mathbf{Q_{32}^\intercal} & \mathbf{Q_{42}^\intercal} \\ \mathbf{Q_{13}^\intercal} & \mathbf{Q_{23}^\intercal} & \mathbf{Q_{33}^\intercal} & \mathbf{Q_{43}^\intercal} \\ \mathbf{Q_{14}^\intercal} & \mathbf{Q_{24}^\intercal} & \mathbf{Q_{34}^\intercal} & \mathbf{Q_{44}^\intercal} \end{bmatrix} \begin{bmatrix} \mathbf{Q_{11}} & \mathbf{Q_{12}} & \mathbf{Q_{13}} & \mathbf{Q_{14}} \\ \mathbf{Q_{21}} & \mathbf{Q_{22}} & \mathbf{Q_{23}} & \mathbf{Q_{24}} \\ \mathbf{Q_{31}} & \mathbf{Q_{32}} & \mathbf{Q_{33}} & \mathbf{Q_{34}} \\ \mathbf{Q_{41}} & \mathbf{Q_{42}} & \mathbf{Q_{43}} & \mathbf{Q_{44}} \end{bmatrix} \\ &= \mathbf{I}, \end{aligned}$$

where $\mathbf{Q_{ij}},\ 1 \leq i, j \leq 4$, are assumed to have the appropriate size. Hence,

$$\begin{aligned} \mathbf{Q_{12}^\intercal Q_{12}} + \mathbf{Q_{22}^\intercal Q_{22}} + \mathbf{Q_{32}^\intercal Q_{32}} + \mathbf{Q_{42}^\intercal Q_{42}} &= \mathbf{I}, \\ \mathbf{Q_{13}^\intercal Q_{13}} + \mathbf{Q_{23}^\intercal Q_{23}} + \mathbf{Q_{33}^\intercal Q_{33}} + \mathbf{Q_{43}^\intercal Q_{43}} &= \mathbf{I}, \end{aligned} \tag{5}$$

$$\mathcal{Q}\mathcal{B}_4 = \begin{bmatrix} \mathbf{0} & \mathbf{Q_{13}}(d'_u + d'_v + 2) & \mathbf{Q_{12}}(d'_u + d'_v + 2) & \mathbf{0} \\ \mathbf{0} & \mathbf{Q_{23}}(d'_u + d'_v + 2) & \mathbf{Q_{22}}(d'_u + d'_v + 2) & \mathbf{0} \\ \mathbf{0} & \mathbf{Q_{33}}(d'_u + d'_v + 2) & \mathbf{Q_{32}}(d'_u + d'_v + 2) & \mathbf{0} \\ \mathbf{0} & \mathbf{Q_{43}}(d'_u + d'_v + 2) & \mathbf{Q_{42}}(d'_u + d'_v + 2) & \mathbf{0} \end{bmatrix}.$$

Since $\mathcal{QB}_4$ is diagonally dominant, we have $\mathbf{Q_{13}} = \mathbf{Q_{12}} = \mathbf{Q_{43}} = \mathbf{Q_{42}} = 0$, as $d'_u + d'_v + 2$ can not be equal to zero. So Equation (5) reduces to

$$\begin{aligned} \mathbf{Q}_{\mathbf{22}}^{\intercal}\mathbf{Q_{22}} + \mathbf{Q}_{\mathbf{32}}^{\intercal}\mathbf{Q_{32}} &= \mathbf{I}, \\ \mathbf{Q}_{\mathbf{23}}^{\intercal}\mathbf{Q_{23}} + \mathbf{Q}_{\mathbf{33}}^{\intercal}\mathbf{Q_{33}} &= \mathbf{I}. \end{aligned} \tag{6}$$

Also,

$$\begin{aligned} \mathcal{QB}_3 &= \begin{bmatrix} \mathbf{Q_{12}}\mathbf{J}_u^{\intercal} & \mathbf{Q_{11}}\mathbf{J}_u & \mathbf{Q_{14}}\mathbf{J}_v & \mathbf{Q_{13}}\mathbf{J}_u^{\intercal} \\ \mathbf{Q_{22}}\mathbf{J}_u^{\intercal} & \mathbf{Q_{21}}\mathbf{J}_u & \mathbf{Q_{24}}\mathbf{J}_v & \mathbf{Q_{23}}\mathbf{J}_u^{\intercal} \\ \mathbf{Q_{32}}\mathbf{J}_u^{\intercal} & \mathbf{Q_{31}}\mathbf{J}_u & \mathbf{Q_{34}}\mathbf{J}_v & \mathbf{Q_{33}}\mathbf{J}_u^{\intercal} \\ \mathbf{Q_{42}}\mathbf{J}_u^{\intercal} & \mathbf{Q_{41}}\mathbf{J}_u & \mathbf{Q_{44}}\mathbf{J}_v & \mathbf{Q_{43}}\mathbf{J}_u^{\intercal} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{0} & \mathbf{Q_{11}}\mathbf{J}_u & \mathbf{Q_{14}}\mathbf{J}_v & \mathbf{0} \\ \mathbf{Q_{22}}\mathbf{J}_u^{\intercal} & \mathbf{Q_{21}}\mathbf{J}_u & \mathbf{Q_{24}}\mathbf{J}_v & \mathbf{Q_{23}}\mathbf{J}_u^{\intercal} \\ \mathbf{Q_{32}}\mathbf{J}_u^{\intercal} & \mathbf{Q_{31}}\mathbf{J}_u & \mathbf{Q_{34}}\mathbf{J}_v & \mathbf{Q_{33}}\mathbf{J}_u^{\intercal} \\ \mathbf{0} & \mathbf{Q_{41}}\mathbf{J}_u & \mathbf{Q_{44}}\mathbf{J}_v & \mathbf{0} \end{bmatrix}, \end{aligned}$$

Again, $\mathbf{Q_{11}}\mathbf{J}_u = \mathbf{Q_{14}}\mathbf{J}_v = \mathbf{Q_{22}}\mathbf{J}_u^{\intercal} = \mathbf{Q_{32}}\mathbf{J}_u^{\intercal} = \mathbf{Q_{41}}\mathbf{J}_u = \mathbf{Q_{44}}\mathbf{J}_v = \mathbf{Q_{33}}\mathbf{J}_u^{\intercal} = \mathbf{Q_{23}}\mathbf{J}_u^{\intercal} = 0$, as $\mathcal{QB}_3$ is also diagonally dominant.
Now, from Equation (6),

$$\begin{aligned} \mathbf{J}_u &= \mathbf{J}_u\mathbf{Q}_{\mathbf{22}}^{\intercal}\mathbf{Q_{22}} + \mathbf{J}_u\mathbf{Q}_{\mathbf{32}}^{\intercal}\mathbf{Q_{32}} \\ &= [\mathbf{Q_{22}}\mathbf{J}_u^{\intercal}]^{\intercal}\mathbf{Q_{22}} + [\mathbf{Q_{32}}\mathbf{J}_u^{\intercal}]^{\intercal}\mathbf{Q_{32}} = \mathbf{0}, \\ \mathbf{J}_v &= \mathbf{J}_v\mathbf{Q}_{\mathbf{23}}^{\intercal}\mathbf{Q_{23}} + \mathbf{J}_v\mathbf{Q}_{\mathbf{33}}^{\intercal}\mathbf{Q_{33}} \\ &= [\mathbf{Q_{23}}\mathbf{J}_v^{\intercal}]^{\intercal}\mathbf{Q_{23}} + [\mathbf{Q_{33}}\mathbf{J}_v^{\intercal}]^{\intercal}\mathbf{Q_{33}} = \mathbf{0}, \end{aligned}$$

which implies both u and v are isolated vertices in Γ_1 and Γ_1 respectively.

Now, it is direct that equality in (3) holds only if the equality in (4) holds and it is direct that, the equality in (3) holds when u and v are isolated vertices in Γ_1 and Γ_2 respectively. Hence the result follows. □

The energy of a graph and a subgraph obtained by deleting an edge is discussed below.

Theorem 8. *Let Γ be a graph and $e = uv$ be an edge in Γ and let d_u and d_v be the degrees of the vertices u and v in the resultant graph $\Gamma - e$. Then*

$$\mathcal{ZE}(\Gamma - e) \geq \mathcal{ZE}(\Gamma) - 2(\sqrt{d_u} + \sqrt{d_v} + d_u + d_v + 2)$$

with equality if and only if $e = uv$ is an isolated edge in Γ.

Proof. Consider

$$\mathcal{Z}^{\Gamma} = \begin{bmatrix} \mathcal{Z}^{\Gamma}[u,v] & [x_1 + x_2] & [y_1 + y_2] \\ [x_1 + x_2]^{\intercal} & \mathbf{0} & d_u + d_v + 2 \\ [y_1 + y_2]^{\intercal} & d_u + d_v + 2 & \mathbf{0} \end{bmatrix},$$

where x_1 and y_1 represents the column vector of $\mathcal{Z}^{\Gamma}$ corresponding to the vertex u and v. The column vector x_2 is obtained by replacing all the non-zero entries of x_1 by -1 and, the column vector y_2 is obtained by replacing all the non-zero entries of y_1 by -1.
The proof follows similarly. □

4. Applications

Pi-electron energy is an important concept in chemistry and material science. It is crucial in describing electron interactions in the pi-orbitals of adjacent atoms in conjugated systems such as double bonds and aromatic rings. These pi-electrons' energy levels have an impact on the stability, reactivity, and electronic properties of organic compounds and conjugated materials. By using the Hückel molecular orbital (HMO) theory one can get many important properties of the conjugated molecules using the total pi-electron energy.

For vinyl compounds specifically, which are organic compounds containing the vinyl functional group (R–CH = CH_2), the Total pi-electron energy would quantify the energy associated with the pi-electrons within the double bond. The Zagreb indices would describe the molecular size and branching patterns of the compound's structure. The pi-electron energy of the polyenes and vinyl compounds [14] are compared with the Zagreb energy and also the scatter plot

is shown in Fig. 1, which shows that the Zagreb energy and pi-electron energy are highly correlated with the correlation coefficient of 0.9971.

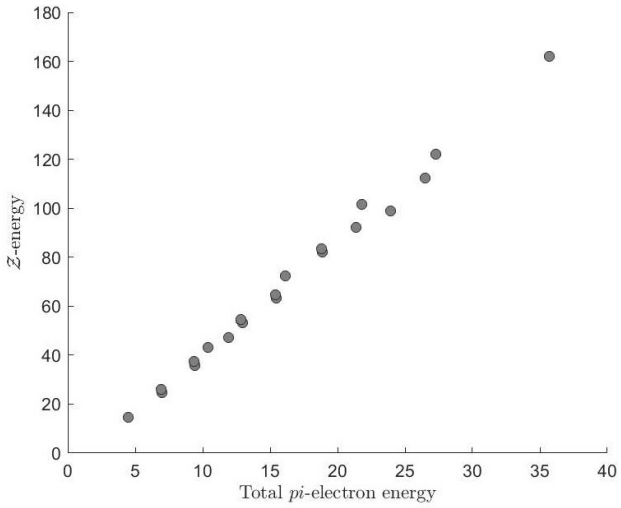

FIG. 1. Scatter plot of total pi-electron energy v/s $\mathcal{Z}$-energy of polyenes and vinyl compounds.

The acentric factor is directly related to the critical properties of a substance, such as its critical temperature and critical pressure. R. Zheng et al. [15], have compared the experimental results of entropy and acentric factor of octane isomers (Fig. 2) with the spectral radius of Arithmetic-Geometric ($\mathcal{AG}$), Atom Bond Connectivity ($\mathcal{ABC}$) and Sombor ($\mathcal{S}$) matrix of the molecular graphs of the same. For octane isomers, they found that correlation coefficient of the spectral radius of $\mathcal{AG}$, $\mathcal{ABC}$ and $\mathcal{S}$ with entropy are -0.917, -0.906 and -0.912, respectively, and with acentric factor it is found to be $-0.947 - 0.930$ and -0.962, respectively.

The acentric factor depends on molecular shape and size, which are influenced by factors such as molecular weight, branching, and symmetry. Alkanes with higher molecular weight and more branching tend to have higher acentric factors because they deviate more from spherical shape and have greater molecular interactions. Entropy is a measure of the number of microscopic configurations or arrangements that are consistent with the macroscopic state of a system. In general, increasing molecular branching tends to increase entropy. This is because branching increases the number of possible arrangements of the molecules, leading to a greater number of microstates accessible to the system. Contrary to this, the spectral radius of graphs (in general) decreases if they deviate more from spherical shape. That is, star graph has the maximum spectral radius ($\sqrt{n-1}$) and path graph has the minimum ($2\cos\frac{\pi}{n+1}$). The correlation study of thermodynamic properties of aromatic compounds with the various topological indices obtained from the eigenvalues of the adjacency matrix has been carried out in [16]. The present study shows that, $\mathcal{Z}$-spectral radius and the acentric factor (entropy) of the octane isomers are negatively correlated with the correlation coefficient of -0.974 (-0.9168). The experimental values of the entropy and acentric factor of octane isomers were taken from [15].

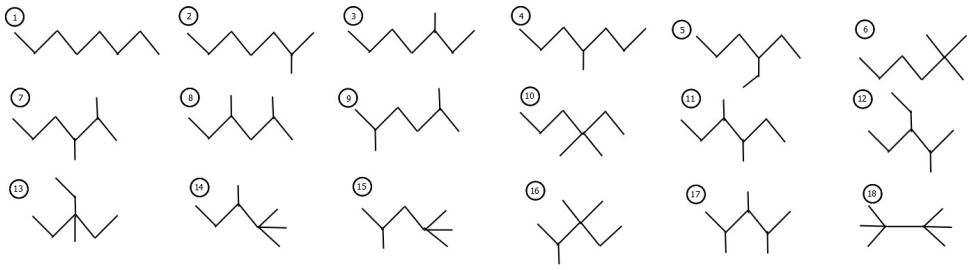

FIG. 2. Octane isomers

Since these factors are well correlated, we can predict the acentric factor and entropy of the octane isomers. Now, from Figs. 6 and 7 we have

$$\text{acenfac} = -0.02172 \times \zeta_1 + 0.5597,$$
$$\text{entropy} = -2.606 \times \zeta_1 + 132.3.$$

The experimental values of density (in g/cm^3), refractive index and acentric factors of the n-alkanes from $C2$ to $C30$ are taken from [17] and from [18–20] and also the $\mathcal{Z}$-spectral radius and $\mathcal{Z}$-energy of the molecular graph of the same has

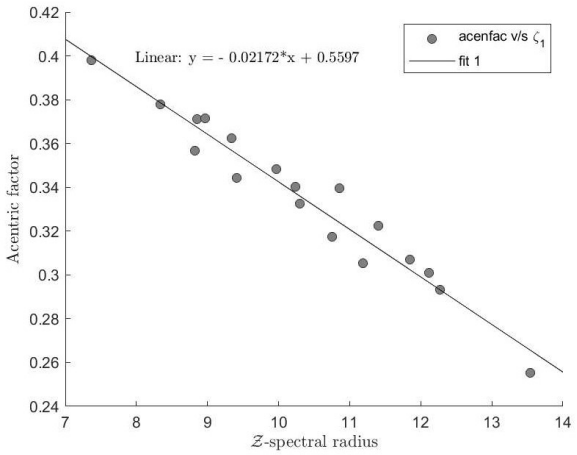

FIG. 3. Linear fit for the scatter plot of acenfac v/s $\mathcal{Z}$-spectral radius.

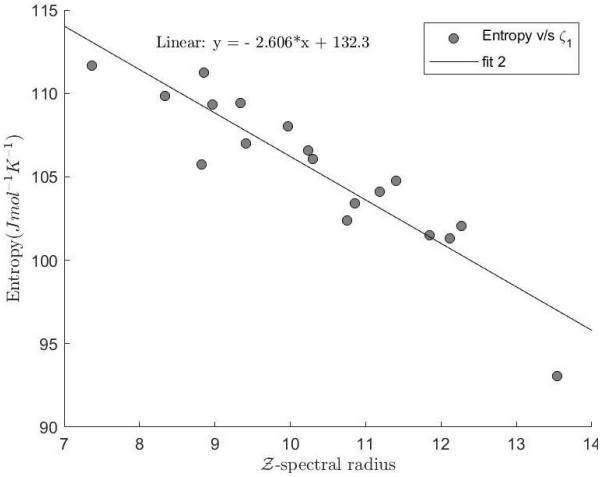

FIG. 4. Linear fit for the scatter plot of entropy v/s $\mathcal{Z}$-spectral radius.

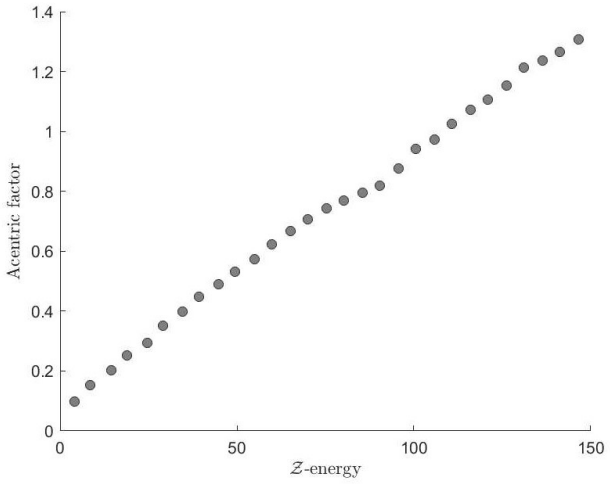

FIG. 5. Scatter plot of acentric factor against Zagreb energy.

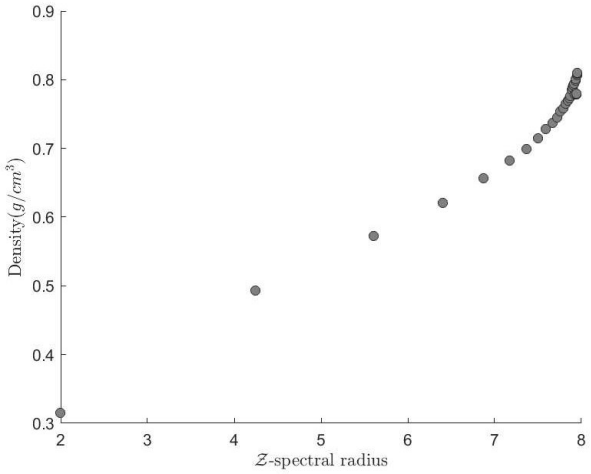

FIG. 6. Scatter plot of density (in gcm^{-3}) against Zagreb spectral radius.

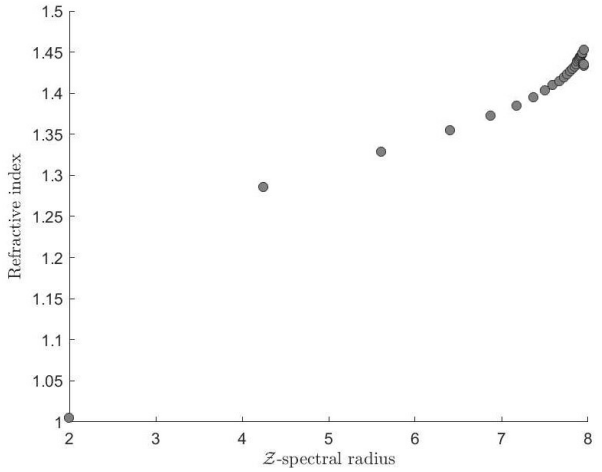

FIG. 7. Scatter plot of refractive index against Zagreb spectral radius.

been computed. Previously, it is observed that the acentric factors of octane isomers are negatively correlated to the $\mathcal{Z}$-spectral radius. Now, a very high positive correlation between the $\mathcal{Z}$-energy and the acentric factor of n-alkanes has been observed, where the correlation coefficient is found to be 0.9989. Even though the branching is similar, the number of carbon atoms are different and more the number of carbon atoms higher the Zagreb energy (of its graphical representation) and also the acentric factor. This increase in acentric factor is because, longer the carbon chain in n-alkanes (i.e., as n increases), more will be the deviation from the spherical shape.

When a molecule is highly branched, it tends to have a lower density compared to a molecule with a linear or less-branched structure. This lower density can lead to a decrease in the refractive index of the material. Hence as expected, it is found that, density and refractive index of the n-alkanes are positively correlated to $\mathcal{Z}$-spectral radius, with respective correlation coefficient of 0.9821 and 0.9693. Figs.5,6 and 7 show that one can predict the acentric factor (and hence the critical properties), density and refractive index of n-alkanes, just by computing the $\mathcal{Z}$-spectral radius and $\mathcal{Z}$-energy.

Conclusion

In this paper, we found some bounds for the spectral radius of the Zagreb matrix of graphs and also we study how it changes during the deletion and rotation of an edge. Also, the change in Zagreb energy of a graph, which is obtained by deleting an edge or identifying the end vertices of an edge, are studied. Mainly, the excellent correlation between the acentric factor (density, refractive index) of n-alkanes and the Zagreb energy (and spectral radius) of the molecular graph of the same has been observed.

References

[1] Gutman I. and Furtula B. *Graph energies and their applications*. Bulletin (Académie serbe des sciences et des arts. Classe des sciences mathématiques et naturelles. Sciences mathématiques), 2019, **44**, P. 29–45.

[2] Gutman I. The energy of a graph. *Ber. Math. Stat. Sekt. Forschungsz. Graz.*, 1978, **103**, P. 1–22.

[3] Bozkurt S.B., A. Dilek G., Gutman I. and Cevik A.S. Randic matrix and Randic energy. *MATCH Commun. Math. Comput. Chem*, 2010, **64**(1), P. 239–250.

[4] Gutman I. and Trinajstić N. Graph theory and molecular orbitals. Total ϕ-electron energy of alternant hydrocarbons. *Chem. phys. lett.*, 1972, **17**(4), P. 535–538.

[5] Gutman I. and Das K.C. The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem.*, 2004, **50**(1), P. 83–92.

[6] Nikolić S., Kovačević G., Miličević A. and Trinajstić N. The Zagreb indices 30 years after. *Croatica Chemica Acta*, 2003, **76**(2), P. 113–124.

[7] Shetty S.S. and Bhat K.A. On the first Zagreb index of graphs with self-loops. *AKCE Inter. J. Graphs Comb.*, 2023, **20**(3), P. 326–331.

[8] Rad N.J., Jahanbani A., and Gutman I. Zagreb energy and Zagreb estrada index of graphs. *MATCH Commun. Math. Comput. Chem.*, 2018, **79**, P. 371–386.

[9] West D.B. *Introduction to graph theory*, **2**. Prentice Hall Upper Saddle River, 2001.

[10] Johnson C.R. and Horn R.A. *Matrix analysis*, Cambridge university press, Cambridge, 1985.

[11] Yuan H. A bound on the spectral radius of graphs. *Linear Algebra Appl*. 1988, **108**, P. 135–139.

[12] Stevanovic D. *Spectral radius of graphs*, Birkhäuser, 2014.

[13] So W., Robbiano M., N.M.M. de Abreu and Gutman I. Applications of theorem by Ky Fan in the theory of graph energy. *Linear Algebra Appl.*, 2010, **432**(9), P. 2163–2169.

[14] Coulson C.A. and Streitwieser A. *Dictionary of π-electron calculations*. Pergamon Press, 1965.

[15] Zheng R., Su P. and Jin X. Arithmetic-geometric matrix of graphs and its applications. *Applied Math. Comput.*, 2023, **442**, P. 371–386.

[16] Hayat S., Mahadi H., Alanazi S. and Wang S. Predictive potential of eigenvalues-based graphical indices for determining thermodynamic properties of polycyclic aromatic hydrocarbons with applications to polyacenes. *Computat. Materials Sci.*, 2024, **238**, P. 112944.

[17] https://www.nist.gov/srd

[18] Ohse R.W. and Tippelskirch H.V. The critical constants of the elements and of some refractory materials with high critical temperatures. *High Temperatures-High Pressures*, 1977, **9**(4), P. 367–385.

[19] Wang Q., Jia Q. and Ma P. Prediction of the acentric factor of organic compounds with the positional distributive contribution method. *Journal of Chemical & Engineering Data*, 2012, **57**(1), P. 169–189.

[20] Yaws C.L. *The yaws handbook of physical properties for hydrocarbons and chemicals: physical properties for more than 54,000 organic and inorganic chemical compounds, Coverage for C1 to C100 Organics and Ac to Zr Inorganics*. Gulf Professional Publishing, 2015.

Submitted 23 January 2024; revised 30 April 2024; accepted 11 May 2024

Information about the authors:

Shashwath S. Shetty – Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, 576104, India; ORCID 0009-0004-0324-1835; shashwathsshetty01334@gmail.com

K. Arathi Bhat – Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, 576104, India; ORCID 0000-0002-1526-5760; arathi.bhat@manipal.edu

Conflict of interest: the authors declare no conflict of interest.