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On the Generalized Vertex Energy of a Graph

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Abstract

The notions of vertex energy and centrality measures are significant graph invariants that describe the contribution of individual vertices to the total energy of graph. Unlike global energy measures, they provide vertex-level information and allow the identification of structurally significant vertices. In this article, we extend the notion of energy of a vertex ($\mathcal{E}_{\mathrm{G}}(v)$) by defining the general vertex degree-based (VDB) vertex energy. Further, we study some particular types

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of this invariant, namely the first Zagreb vertex energy ($\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$), second Zagreb vertex energy ($\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$), forgotten vertex energy ($\mathcal{F}\mathcal{E}_{\mathrm{G}}(v)$), Sombor vertex energy ($\mathcal{SOE}_{\mathrm{G}}(v)$) and atom-bond connectivity vertex energy ($\mathcal{ABCE}_{\mathrm{G}}(v)$), derived from the corresponding VDB topological indices and their associated VDB index-weighted adjacency matrices. Furthermore, using the method proposed by Arizmendi *et* al., we compute these invariants for certain standard graphs. Subsequently, we perform a vertex-level regression analysis between the eigenvector centrality measure ($\mathcal{X}_i$) and these particular VDB vertex energy invariants, with reference to each of the 18 octane isomers, through which we observe a strong correlation between these parameters, thereby establishing their significance.

1 Introduction

Chemical graph theory constitutes an important area of mathematical chemistry in which graph theoretical principles are employed to analyze molecular structures. In this approach, a molecule is modeled as a graph $\mathrm{G}(\mathrm{V}, \mathrm{E})$, where the vertex set V represents atoms and the edge set E represents chemical bonds. The order of G corresponds to the number of atoms, while its size corresponds to the number of bonds. In a graph G, two vertices are said to be adjacent if the corresponding atoms are joined by a chemical bond. The resulting molecular (skeletal) graph captures the essential bonding pattern of the compound and enables the investigation of important molecular properties such as connectivity, symmetry, stability and chemical reactivity. In recent years, chemical graph theory has found applications in diverse areas including chemistry, biology, ecology, sociology, computer science, discrete mathematics and statistics.

An important concept in this domain is the notion of topological indices that depend exclusively on the structure of the associated molecular graph. A topological index is a numerical quantity derived from molecular graphs designed to characterize structural features of a molecule and to establish correlations with its physico-chemical properties, biological activities and chemical reactivity. Several molecular characteristics such as toughness, melting point, entropy, rigidity, boiling point, strain energy, enthalpy of formation and enthalpy of vaporization are known to be closely associated with the underlying graphical structure of chemical compounds. Hence, they play a significant role in QSPR/QSAR investigations and molecular modeling.

Among various classes of topological indices, vertex degree-based topological indices occupy a prominent position. These indices can be generally expressed as

$$TI(\mathrm{G}) = \sum_{v_iv_j \in \mathrm{E(G)}} f(d(v_i), d(v_j)),$$

where $f(d(v_i), d(v_j))$ is a symmetric function of the end vertices of each edge v_iv_j. Here, $d(v_i)$ and $d(v_j)$ denote the degree of the vertices v_i and v_j respectively. Some of the well known VDB topological indices are Zagreb index [26], Randić index [42], Sombor index [15], forgotten index [26] and atom-bond connectivity index [17]. These descriptors effectively capture degree related structural information and have been widely investigated in theoretical and applied studies.

In addition to VDB topological invariants, spectral descriptors provide another important direction in chemical graph theory. Among them, graph energy has emerged as a significant spectral descriptor. It was first introduced by Gutman [23] in 1978, motivated by the results concerning the total π-electron energy in Hückel molecular orbital theory. The energy of a simple graph G with adjacency matrix $\mathcal{A}(\mathrm{G})$ and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ is defined as

$$\mathcal{E}(\mathrm{G}) = \sum_{i=1}^{n} |\lambda_i|.$$

Since eigenvalues reflect fundamental structural characteristics of graphs, graph energy also provides valuable insight into their intrinsic properties. Consequently, graph energy has attracted significant attention in both pure and applied mathematics. Over the years, extensive research has been carried out on the energy of graphs and its invariants. These energy invariants establish a meaningful connection between structural descriptors and eigenvalue based analysis, thereby enriching both theoretical investigations and practical applications. They have applications in diverse areas such as crystallography, air transportation, satellite communication, face, pattern and object recognition, spacecraft construction and QSPR/QSAR analysis of drug molecules [32,34]. Various types of graph energies have been introduced and investigated in literature [5,18,19,25,27,48,61]. Some notable invariants include Zagreb energy, Randić energy, atom-bond connectivity energy, Sombor energy and forgotten energy.

Thus, topological indices and graph energy invariants have received considerable attention as several physico-chemical properties can be observed directly from molecular structures without requiring experimental efforts. This makes them useful tools for QSPR/QSAR studies in molecular design. However, most existing VDB topological indices and graph energy invariants have inherent limitations, including poor representations of multiple bonds, hetero atoms and molecular spatial arrangements. In addition, these descriptors usually provide a global characterization of molecules, emphasizing overall size or shape, rather than capturing individual contributions of distinct atomic types or functional groups. Although such local features play a decisive role in intermolecular interactions and physico-chemical behavior, they are not explicitly reflected in conventional topological indies and energy invariants. As a result, the effectiveness of correlating these descriptors with physical properties or biological activities, particularly in pharmaceutical molecules, remains limited.

In order to overcome these limitations, the local version of graph energy, called the energy of a vertex has been introduced in spectral graph theory. This notion quantifies the contribution of an individual vertex to the total energy of a graph, thereby enabling vertex-level structural analysis. The concept was first proposed by Arizmendi *et* al. [2]. For a given vertex v_i, the energy of a vertex is defined as

$$\mathcal{E}_{\mathrm{G}}(v_i) = |\mathcal{A}(\mathrm{G})|_{ii} \text{ for } i = 1, 2, \ldots, n,$$

where $|\mathcal{A}| = (\mathcal{A}\mathcal{A}^*)^{\frac{1}{2}}$ and $\mathcal{A}^*$ is the conjugate transpose of the adjacency matrix. This quantity satisfies the additional property

$$\mathcal{E}(\mathrm{G}) = \sum_{i=1}^{n} \mathcal{E}_{\mathrm{G}}(v_i).$$

Thus, vertex energy provides a bridge between the global spectral invariants and the local structural contributions.

In general, the distribution of vertex energy is closely related to structural symmetry and in particular, it is associated with vertex symmetry, a fundamental structural property of graphs that reflects their internal uniformity. A graph is called vertex transitive if for any pair of vertices v_i and v_j, there exist an automorphism ϕ such that $\phi(v_i) = v_j$, where an automorphism is a bijective adjacency preserving mapping. Consequently, all vertices are structurally equivalent and interchangeable. In spectral graph theory, vertex symmetry ensures that eigenvalue-related characteristics are uniform throughout the graph. Well known examples of vertex transitive graphs include complete graph, cycle graph, peterson graph, hypercubes and Cayley graphs.

Vertex energy has been investigated for many classes of graphs, including complete graphs, paths, cycles, hypercubes, complete bipartite graphs, subdivision graphs, non isomorphic integral trees (order up to 30), non-regular non-bipartite integral graphs with maximum vertex degree four, integral trees and other highly symmetric or regular structures [2, 4, 35, 38, 41, 49–51]. Spectral techniques, particularly eigenvector-based approaches [2,3,24,41], have been employed to examine the influence of symmetry, regularity and graph operations on vertex energy distributions. Furthermore, the behavior of vertex energy under graph transformations and its variation in special classes of trees and bipartite graphs have also been examined, highlighting the importance of structural properties in determining vertex-level energy distributions [4,14]. Also, Randić vertex energy, a modified version of the vertex energy based on the Randić index and the associated Randić matrix has been introduced and studied in recent literature [21].

On the other hand, centrality is a fundamental concept in network analysis and has received increasing attention in chemical graph theory. Initially introduced to explain variations in communication network performance such as problems of solving time, error rates, leadership recognition, efficiency and job distribution, in recent years, centrality measures have been widely applied to complex networks composed of nodes and links in diverse fields, including physics, biology and social sciences. Identifying important or influential nodes in such networks is crucial for understanding information flow and dynamic processes. Consequently, centrality serves as a quantitative indicator of node importance and has become an effective tool for the analysis of complex networks and the characterization of chemical structures.

Centrality measures are broadly categorized into local and global categories. Centrality measures that can be calculated by using only immediate neighborhood of node are called local centrality measures. Degree centrality measure and semilocal centrality measure have been considered as local centrality measures. In contrast, global centrality measures such as closeness centrality, betweenness centrality, eigenvector centrality, coreness centrality, page rank etc. require knowledge of entire structure of the network and therefore involve higher computational complexity.

The centrality measures such as degree, closeness, betweenness and eigenvector centrality measures are based on the shortest paths between pairs of entities, quantifying the number of paths that pass through a specific vertex. By employing suitable centrality measures, the structural significance of individual atoms and their relationships within a molecular graph can also be quantified. As a result, centrality measures serve as effective descriptors for QSPR/QSAR analysis. Due to their theoretical relevance and practical applications, these centrality measures have been extensively investigated in literature [6–11,29,30,33,37,43,47,52–54,56,58–60,62]. Together, vertex energy and centrality measures facilitate detailed atomic level investigations of molecular structures and chemical networks.

Inspired by the work carried out as discussed above, in the present work, we aim to perform a vertex-level spectral analysis by means of introducing the general VDB vertex energy, based on VDB indices $TI(\mathrm{G})$ of a graph G. Further, we study some of the particular VDB vertex energies such as the first Zagreb vertex energy ($\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$), second Zagreb vertex energy ($\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$), forgotten vertex energy ($\mathcal{F}\mathcal{E}_{\mathrm{G}}(v)$), Sombor vertex energy ($\mathcal{S}\mathcal{O}\mathcal{E}_{\mathrm{G}}(v)$) and atom-bond connectivity vertex energy ($\mathcal{A}\mathcal{B}\mathcal{C}\mathcal{E}_{\mathrm{G}}(v)$), defined through their corresponding VDB topological indices and their associated VDB index-weighted adjacency matrices. We also compute these vertex energy invariants for selected standard graphs using the method proposed in [2, 21]. Furthermore, to explore the structural relevance of these newly defined invariants, we study their relationship with centrality measures, particularly with eigenvector centrality measure. Also, a vertex-level regression analysis is carried out on octane isomers to examine the correlation between eigenvector centrality measure and the proposed VDB vertex energy invariants. Through this approach, we aim to establish a relationship between vertex energy invariants and the centrality based structural measures within molecular graphs.

2 Preliminaries

Throughout the paper, G denotes a non-trivial connected simple graph. The vertex set of G is denoted by V(G) $= \{v_1, v_2, \ldots, v_n\}$ and the edge set is denoted by E(G) $= \{e_1, e_2, \ldots, e_m\}$. The degree of a vertex v_i in G is represented by $d(v_i)$. $M_n(\mathbb{C})$ denotes the set of all $n \times n$ matrices with complex entries. For $\mathcal{N} \in M_n(\mathbb{C})$, the absolute value of $\mathcal{N}$ is denoted by $|\mathcal{N}| = (\mathcal{N}\mathcal{N}^*)^{\frac{1}{2}}$, where $\mathcal{N}^*$ is the conjugate transpose of $\mathcal{N}$. In the study, $\mathcal{N}$ denotes the VDB index-weighted adjacency matrix constructed by replacing the adjacency matrix $\mathcal{A}$(G) with the matrix based on the general VDB topological index. In particular, we study the matrices associated with the VDB topological indices, namely the first Zagreb index, second Zagreb index, forgotten index, Sombor index and atom-bond connectivity index, whose formal definitions are provided in Table 1.

Topological index	**Mathematical expression**
$\mathcal{M}_1(\mathrm{G})$	$\sum_{v_iv_j \in \mathrm{E(G)}} (d(v_i) + d(v_j))$
$\mathcal{M}_2(\mathrm{G})$	$\sum_{v_iv_j \in \mathrm{E(G)}} (d(v_i) \cdot d(v_j))$
$\mathcal{F}(\mathrm{G})$	$\sum_{v_iv_j \in \mathrm{E(G)}} \left(d(v_i)^2 + d(v_j)^2\right)$
$\mathcal{SO}(\mathrm{G})$	$\sum_{v_iv_j \in \mathrm{E(G)}} \sqrt{d(v_i)^2 + d(v_j)^2}$
$\mathcal{ABC}(\mathrm{G})$	$\sum_{v_iv_j \in \mathrm{E(G)}} \sqrt{\frac{d(v_i) + d(v_j) - 2}{d(v_i) \cdot d(v_j)}}$

Table 1. Definition of VDB topological indices

The adjacency matrix of G is given by $\mathcal{A}(\mathrm{G}) = (a_{ij})_{n\times n}$, where

$$a_{ij} = \begin{cases} 1 & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise.} \end{cases}$$

The energy of a graph G is defined as the sum of the absolute values of the eigenvalues of $\mathcal{A}(\mathrm{G})$.

In a similar manner, the matrix associated with the general VDB index $TI(\mathrm{G})$, called the general VDB index-weighted adjacency matrix, is defined as

$$\mathcal{N}(\mathrm{G}) = (m_{ij})$$

where

$$m_{ij} = \begin{cases} f(d(v_i), d(v_j)) & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise} \end{cases}$$

and

$$TI(\mathrm{G}) = \sum_{v_iv_j \in \mathrm{E(G)}} f(d(v_i), d(v_j)).$$

In particular, we have some of the VDB index-weighted adjacency matrices, derived from the respective VDB topological indices, mentioned in Table 1, as provided in Table 2.

Matrix	**Notation**	**Definition**
First Zagreb matrix	$\mathcal{N}_{\mathcal{M}_1}(\mathrm{G})$ [26]	$m_{ij} = \begin{cases} d(v_i) + d(v_j) & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise.} \end{cases}$
Second Zagreb matrix	$\mathcal{N}_{\mathcal{M}_2}(\mathrm{G})$ [26]	$m_{ij} = \begin{cases} d(v_i) \cdot d(v_j) & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise.} \end{cases}$
Forgotten matrix	$\mathcal{N}_{\mathcal{F}}(\mathrm{G})$	$m_{ij} = \begin{cases} d(v_i)^2 + d(v_j)^2 & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise.} \end{cases}$
Sombor matrix	$\mathcal{N}_{\mathcal{S}}(\mathrm{G})$ [22]	$m_{ij} = \begin{cases} \sqrt{d(v_i)^2 + d(v_j)^2} & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise.} \end{cases}$
ABC matrix	$\mathcal{N}_{\mathcal{ABC}}(\mathrm{G})$ [20]	$m_{ij} = \begin{cases} \sqrt{\frac{d(v_i)+d(v_j)-2}{d(v_i)\cdot d(v_j)}} & \text{if } v_iv_j \in \mathrm{E(G)}, \\ 0 & \text{otherwise.} \end{cases}$

Table 2. Definition of VDB index-weighted adjacency matrices based on the corresponding VDB topological indices

For each matrix, the sum of the absolute values of its eigenvalues defines the corresponding topological index-based energy of the graph G.

Methodology

The general methodology adopted in this study is based on the approach proposed in [2, 21], which is outlined below:

Let ϕ_i be a positive linear functional $\phi_i : M_n(\mathbb{C}) \mapsto \mathbb{C}$, defined for a graph G by $\phi_i(\mathcal{N}(\mathrm{G})) \mapsto \mathcal{N}(\mathrm{G})_{ii}$, where $\mathcal{N}$ denotes a VDB index-weighted adjacency matrix constructed by modifying the adjacency matrix $\mathcal{A}(\mathrm{G})$ through degree based topological indices. Using this functional, the trace of the matrix $\mathcal{N}(\mathrm{G})$ can be expressed as

$$\mathrm{trace}(\mathcal{N}(\mathrm{G})) = \phi_1(\mathcal{N}(\mathrm{G})) + \phi_2(\mathcal{N}(\mathrm{G})) + \cdots + \phi_n(\mathcal{N}(\mathrm{G})).$$

The vertex energy, corresponding to the vertex v_i, is then defined as

$$\mathcal{N}\mathcal{E}_{\mathrm{G}}(v_i) = \phi_i(|\mathcal{N}(\mathrm{G})|) = |\mathcal{N}(\mathrm{G})|_{ii},$$

where $|\mathcal{N}(\mathrm{G})| = (\mathcal{N}(\mathrm{G})\mathcal{N}(\mathrm{G})^*)^{1/2}$ is the absolute value of $\mathcal{N}(\mathrm{G})$.

Consequently,

$$\mathrm{trace}(|\mathcal{N}(\mathrm{G})|) = \phi_1(|\mathcal{N}(\mathrm{G})|) + \phi_2(|\mathcal{N}(\mathrm{G})|) + \cdots + \phi_n(|\mathcal{N}(\mathrm{G})|),$$

so that

$$\mathcal{N}\mathcal{E}(G) = \mathcal{N}\mathcal{E}_{\mathrm{G}}(v_1) + \mathcal{N}\mathcal{E}_{\mathrm{G}}(v_2) + \cdots + \mathcal{N}\mathcal{E}_{\mathrm{G}}(v_n) = \sum_{i=1}^{n} \mathcal{N}\mathcal{E}_{\mathrm{G}}(v_i).$$

For the matrix $\mathcal{N}(\mathrm{G})$, the following result holds. Its proof follows the arguments similar to those used in the proof of Lemma 2.1 of [21].

Lemma 1. *Let* G *be a graph of order* n*. Then,*

$$|\mathcal{N}(\mathrm{G})|_{ii} = \mathcal{N}\mathcal{E}_G(v_i) = \sum_{j=1}^{n} p_{ij}\, |\eta_j| \,, \quad i = 1, \ldots, n,$$

where η_j denotes the j^{th} eigenvalue of $\mathcal{N}(\mathrm{G})$ and

$$\sum_{i=1}^{n} p_{ij} = 1 \qquad and \qquad \sum_{j=1}^{n} p_{ij} = 1.$$

Further, $p_{ij} = y_{ij}^2$, where $Y = (y_{ij})$ is the matrix of orthonormal vectors of the eigenvectors of $\mathcal{N}(\mathrm{G})$.

As a consequence of Lemma 1, we obtain

$$|\mathcal{N}(\mathrm{G})|_{ii} = \sum_{j=1}^{n} y_{ij}^2 \, |\eta_j| \, ,$$

so that

$$\mathcal{N}\mathcal{E}_G(v_i) = \sum_{j=1}^{n} y_{ij}^2 \, |\eta_j| \, .$$

This result holds for any VDB index-weighted adjacency matrix $\mathcal{N}(\mathrm{G})$ corresponding to any VDB topological index.

Lemma 2. *Let $\phi_i : M_n(\mathbb{C}) \mapsto \mathbb{C}$ be a positive map, defined for a graph* G *by $\phi_i(\mathcal{N}(\mathrm{G})) \mapsto \mathcal{N}(\mathrm{G})_{ii}$. Then,*

$$\phi_i\left(\mathcal{N}^k(\mathrm{G})\right) = \sum_{j=1}^{n} y_{ij}^2 \left(\eta_j^k\right), \qquad i = 1, \ldots, n,$$

where $Y = (y_{ij})$ is as described earlier.

As discussed in [49], for a graph G with k distinct eigenvalues $\eta_1, \ldots, \eta_k$ and r vertex symmetries, the vertex set of G can be partitioned into r classes, each consisting of vertices with identical vertex energies. By Lemma 1, these vertex energies can be determined by solving r systems of k linear equations in k unknowns of the form

$$\begin{aligned} p_{i1} + p_{i2} + \cdots + p_{ik} &= \phi_i(1) \\ p_{i1}\eta_1 + p_{i2}\eta_2 + \cdots + p_{ik}\eta_k &= \phi_i(\mathcal{N}) \\ p_{i1}\eta_1^2 + p_{i2}\eta_2^2 + \cdots + p_{ik}\eta_k^2 &= \phi_i(\mathcal{N}^2) \\ \vdots \qquad \vdots \qquad &\vdots \end{aligned}$$

$$p_{i1}\eta_1^{k-1} + p_{i2}\eta_2^{k-1} + \cdots + p_{ik}\eta_k^{k-1} = \phi_i(\mathcal{N}^{k-1}).$$

Thus, if

$$J = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \eta_1 & \eta_2 & \cdots & \eta_k \\ \eta_1^2 & \eta_2^2 & \cdots & \eta_k^2 \\ \vdots & \vdots & \vdots & \vdots \\ \eta_1^{k-1} & \eta_2^{k-1} & \cdots & \eta_k^{k-1} \end{pmatrix}$$

,

$$P = \begin{pmatrix} p_{11} & p_{21} & \cdots & p_{r1} \\ p_{12} & p_{22} & \cdots & p_{r2} \\ \vdots & \vdots & \vdots & \vdots \\ p_{1k} & p_{2k} & \cdots & p_{rk} \end{pmatrix}$$

and

$$Y = \begin{pmatrix} \phi_1(1) & \phi_2(1) & \cdots & \phi_r(1) \\ \phi_1(\mathcal{N}) & \phi_2(\mathcal{N}) & \cdots & \phi_r(\mathcal{N}) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(\mathcal{N}^{k-1}) & \phi_2(\mathcal{N}^{k-1}) & \cdots & \phi_r(\mathcal{N}^{k-1}) \end{pmatrix},$$

then, the complete system can be written as

$$JP = Y.$$

Since J is non-singular, the unique solution of the system is given by

$$P = J^{-1}Y.$$

Using this formulation, the vertex energies corresponding to each symmetry class can be computed.

Remark. It is observed that for graphs having single edge partition, such as the complete graph, complete bipartite graph, star graph, cycle graph and $r-$regular graph, all edges contribute the same weight α_{G}. Hence, the VDB index-weighted adjacency matrix $\mathcal{N}(\mathrm{G})$ can be written as $\mathcal{N}(\mathrm{G}) = \alpha_{\mathrm{G}} \cdot \mathcal{A}(\mathrm{G})$. Consequently, for such graphs, the above systems can be rewritten as

$$\begin{aligned} p_{i1}+p_{i2}+\cdots+p_{ik} &= \phi_i(1)\\ p_{i1}\eta_1+p_{i2}\eta_2+\cdots+p_{ik}\eta_k &= \alpha_{\mathrm{G}}\cdot\phi_i(\mathcal{A})\\ p_{i1}\eta_1^2+p_{i2}\eta_2^2+\cdots+p_{ik}\eta_k^2 &= \alpha_{\mathrm{G}}^2\cdot\phi_i(\mathcal{A}^2)\\ \vdots \qquad\quad \vdots \qquad\quad & \vdots\\ p_{i1}\eta_1^{k-1}+p_{i2}\eta_2^{k-1}+\cdots+p_{ik}\eta_k^{k-1} &= \alpha_{\mathrm{G}}^{k-1}\cdot\phi_i(\mathcal{A}^{k-1}), \end{aligned}$$

where $\phi_i\left(\mathcal{A}^j\right)$ represents the number of $v_i - v_i$ walks of G of length j, $j=1,\dots,k-1$, for each $i=1,2,\dots,r$.

3 Results

Theorem 1. *For the complete graph* $\mathrm{G}=K_n$*, the general VDB vertex energy is given by*

$$\mathcal{NE}_{K_n}(v)=\frac{2f(n-1,n-1)(n-1)}{n},$$

where $f(n-1,n-1)$ *is the value of the associated weight function corresponding to the VDB topological index for* K_n*.*

Proof. The complete graph K_n consists of n vertices with each vertex of degree $n-1$. For any VDB topological index, the corresponding VDB index-weighted adjacency matrix of K_n has the spectrum $\{-f(n-1,n-1)^{n-1}, f(n-1,n-1)(n-1)^1\}$, which gives the total energy $\mathcal{NE}(K_n)=2f(n-1,n-1)(n-1)$.

Since K_n is vertex transitive, every vertex is structurally equivalent and hence has the same vertex energy. Therefore,

$$\mathcal{NE}_{K_n}(v)=\frac{2f(n-1,n-1)(n-1)}{n}\,. \qquad \blacksquare$$

As a direct consequence, we have the following result.

Corollary 1. *The VDB vertex energies of* $\mathrm{G}=K_n$ *corresponding to* $\mathcal{M}_1(\mathrm{G})$*,* $\mathcal{M}_2(\mathrm{G})$*,* $\mathcal{F}(\mathrm{G})$*,* $\mathcal{SO}(\mathrm{G})$ *and* $\mathcal{ABC}(\mathrm{G})$ *are listed as follows:*

Vertex energy invariant	**VDB vertex energy**
$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$\frac{4(n-1)^2}{n}$
$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$\frac{2(n-1)^3}{n}$
$\mathcal{F}\mathcal{E}_{\mathrm{G}}(v)$	$\frac{4(n-1)^3}{n}$
$\mathcal{SO}\mathcal{E}_{\mathrm{G}}(v)$	$\frac{2\sqrt{2}(n-1)^2}{n}$
$\mathcal{ABC}\mathcal{E}_{\mathrm{G}}(v)$	$\frac{2\sqrt{2}\sqrt{n-2}}{n}$

Table 3. VDB vertex energy for each vertex in K_n

Lemma 3. *[2] Let* G *be a bipartite graph with parts* V_1 *and* V_2*. Then,* $\sum\limits_{v\in \mathrm{V}_1} \mathcal{E}_{\mathrm{G}}(v) = \sum\limits_{v\in \mathrm{V}_2} \mathcal{E}_{\mathrm{G}}(v)$.

Theorem 2. *For the complete bipartite graph* $\mathrm{G} = K_{m,n}$ *having disjoint vertex partitions* V_1 *and* V_2 *with* $|\mathrm{V}_1| = m$ *and* $|\mathrm{V}_2| = n$*, the general VDB vertex energy is given by*

$$\mathcal{NE}_{K_{m,n}}(v) = \begin{cases} f(m,n)\dfrac{\sqrt{n}}{\sqrt{m}} & \text{if } v \in \mathrm{V}_1, \\ f(m,n)\dfrac{\sqrt{m}}{\sqrt{n}} & \text{if } v \in \mathrm{V}_2. \end{cases}$$

where $f(m,n)$ *is the value of the associated weight function corresponding to the VDB topological index for* $K_{m,n}$*.*

Proof. The complete bipartite graph $K_{m,n}$ consists of two distinct vertex sets V_1 and V_2 with $|\mathrm{V}_1| = m$ and $|\mathrm{V}_2| = n$. Each vertex in V_1 is adjacent to all n vertices of V_2 and each vertex in V_2 is adjacent to all m vertices of V_1.

For any VDB topological index, the corresponding VDB index-weighted adjacency matrix of $K_{m,n}$ has the spectrum $\{0^{m+n-2}, \pm f(m,n)\sqrt{mn}\}$, which gives the total energy $\mathcal{NE}(K_{m,n}) = 2f(m,n)\sqrt{mn}$.

Since $K_{m,n}$ is edge transitive, all vertices within the same partition are structurally equivalent. Hence, all vertices within the same partition share the same vertex energy.

From Lemma 3, we see that the contribution of each part is proportional to the size of the opposite part. Consequently, each vertex $v_i \in \mathrm{V}_1$ has the energy $\mathcal{E}_{K_{m,n}}(v_i) = f(m,n)\frac{\sqrt{mn}}{n}$. Similarly, each vertex $v_i \in \mathrm{V}_2$, has the energy $\mathcal{E}_{K_{m,n}}(v_i) = f(m,n)\frac{\sqrt{mn}}{m}$.
Hence,

$$\mathcal{NE}_{K_{m,n}}(v) = \begin{cases} f(m,n)\dfrac{\sqrt{n}}{\sqrt{m}} & \text{if } v \in \mathrm{V}_1, \\ f(m,n)\dfrac{\sqrt{m}}{\sqrt{n}} & \text{if } v \in \mathrm{V}_2. \end{cases} \qquad \blacksquare$$

As a consequence of Theorem 2, we obtain the following result.

Corollary 2. *The VDB vertex energy of* $\mathrm{G} = K_{m,n}$ *corresponding to* $\mathcal{M}_1(\mathrm{G})$, $\mathcal{M}_2(\mathrm{G})$, $\mathcal{F}(\mathrm{G})$, $\mathcal{SO}(\mathrm{G})$ *and* $\mathcal{ABC}(\mathrm{G})$ *are listed as follows:*

Vertex energy invariant	**VDB vertex energy**	
	$\boldsymbol{v \in \mathrm{V}_1}$	$\boldsymbol{v \in \mathrm{V}_2}$
$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$m+n\frac{\sqrt{n}}{\sqrt{m}}$	$m+n\frac{\sqrt{m}}{\sqrt{n}}$
$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$mn\frac{\sqrt{n}}{\sqrt{m}}$	$mn\frac{\sqrt{m}}{\sqrt{n}}$
$\mathcal{FE}_{\mathrm{G}}(v)$	$m^2+n^2\frac{\sqrt{n}}{\sqrt{m}}$	$m^2+n^2\frac{\sqrt{m}}{\sqrt{n}}$
$\mathcal{SOE}_{\mathrm{G}}(v)$	$\sqrt{m^2+n^2}\frac{\sqrt{n}}{\sqrt{m}}$	$\sqrt{m^2+n^2}\frac{\sqrt{m}}{\sqrt{n}}$
$\mathcal{ABCE}_{\mathrm{G}}(v)$	$\frac{\sqrt{m+n-2}}{m}$	$\frac{\sqrt{m+n-2}}{n}$

Table 4. VDB vertex energy for each vertex in $K_{m,n}$ with partitions V_1 and V_2

Theorem 3. *For the cycle graph* $\mathrm{G} = C_n$*, the general VDB vertex energy is given by*

$$\mathcal{NE}_G(v) = \begin{cases} f(2,2)\dfrac{4cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})} & \textit{if } n \equiv 0\,(mod\ 4), \\ f(2,2)\dfrac{4}{nsin(\frac{\pi}{n})} & \textit{if } n \equiv 2\,(mod\ 4), \\ f(2,2)\dfrac{2}{nsin(\frac{\pi}{2n})} & \textit{if } n \equiv 1\,(mod\ 2), \end{cases}$$

where $f(2,2)$ *is the value of the associated weight function corresponding to the VDB topological index for* C_n.

Proof. The cycle graph C_n consists of n vertices, each vertex has degree 2. For any VDB topological index, the corresponding VDB index-weighted adjacency matrix of C_n has the spectrum $\{2f(2,2)cos(\frac{2k\pi}{n}) \mid k \in \{0,1,2,\dots,n-1\}\}$, which gives the total energy $\sum_{k=0}^{n-1}\left|2f(2,2)cos\left(\frac{2k\pi}{n}\right)\right|$.

For the cycle graph C_n of order $n \geq 3$, the total energy depends on the residue class of n and is given by

$$\mathcal{NE}(C_n) = \begin{cases} f(2,2)\dfrac{4cos(\frac{\pi}{n})}{sin(\frac{\pi}{n})} & \text{if } n \equiv 0\,(mod\ 4), \\ f(2,2)\dfrac{4}{sin(\frac{\pi}{n})} & \text{if } n \equiv 2\,(mod\ 4), \\ f(2,2)\dfrac{2}{sin(\frac{\pi}{2n})} & \text{if } n \equiv 1\,(mod\ 2). \end{cases}$$

Since C_n is vertex transitive, all its vertices have same energy. Thus, the vertex energy, corresponding to each $n \geq 3$, is given by

$$\mathcal{NE}_G(v) = \begin{cases} f(2,2)\dfrac{4cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})} & \text{if } n \equiv 0\,(mod\ 4), \\ f(2,2)\dfrac{4}{nsin(\frac{\pi}{n})} & \text{if } n \equiv 2\,(mod\ 4), \\ f(2,2)\dfrac{2}{nsin(\frac{\pi}{2n})} & \text{if } n \equiv 1\,(mod\ 2). \end{cases} \qquad \blacksquare$$

As a consequence of Theorem 3, we obtain the following result.

Corollary 3. *The VDB vertex energy of* $\mathrm{G} = C_n$ *corresponding to* $\mathcal{M}_1(\mathrm{G})$, $\mathcal{M}_2(\mathrm{G})$, $\mathcal{F}(\mathrm{G})$, $\mathcal{SO}(\mathrm{G})$ *and* $\mathcal{ABC}(\mathrm{G})$ *are listed as follows:*

4 Regression analysis

Regression analysis investigates the relationship between an independent variable X and a dependent variable Y by representing Y as an n^{th} degree polynomial function of X. This framework facilitates the modeling of both linear and non-linear relationships between predictor and response variable. The primary objective of regression analysis is to estimate or predict the expected value of a dependent variable Y based on the corresponding value of the independent variable X. In chemical graph theory,

Invariant	**VDB vertex energy**		
	$\boldsymbol{n \equiv 0\,(mod\ 4)}$	$\boldsymbol{n \equiv 2\,(mod\ 4)}$	$\boldsymbol{n \equiv 1\,(mod\ 2)}$
$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$\dfrac{16\,cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})}$	$\dfrac{16}{nsin(\frac{\pi}{n})}$	$\dfrac{8}{nsin(\frac{\pi}{2n})}$
$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$\dfrac{16\,cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})}$	$\dfrac{16}{nsin(\frac{\pi}{n})}$	$\dfrac{8}{nsin(\frac{\pi}{2n})}$
$\mathcal{F}\mathcal{E}_{\mathrm{G}}(v)$	$\dfrac{32\,cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})}$	$\dfrac{32}{nsin(\frac{\pi}{n})}$	$\dfrac{16}{nsin(\frac{\pi}{2n})}$
$\mathcal{S}\mathcal{O}\mathcal{E}_{\mathrm{G}}(v)$	$\dfrac{8\sqrt{2}\,cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})}$	$\dfrac{8\sqrt{2}}{nsin(\frac{\pi}{n})}$	$\dfrac{4\sqrt{2}}{nsin(\frac{\pi}{2n})}$
$\mathcal{A}\mathcal{B}\mathcal{C}\mathcal{E}_{\mathrm{G}}(v)$	$\dfrac{2\sqrt{2}\,cos(\frac{\pi}{n})}{nsin(\frac{\pi}{n})}$	$\dfrac{2\sqrt{2}}{nsin(\frac{\pi}{n})}$	$\dfrac{\sqrt{2}}{nsin(\frac{\pi}{2n})}$

Table 5. VDB vertex energy for each vertex in C_n

regression methods are extensively employed to model and predict various chemical, physical and biological properties of molecules through their graph-theoretic representations. Consequently, regression models provide a powerful mathematical tool for structural interpretation and property prediction based on molecular descriptors. Commonly employed regression models are given below.

$$\begin{aligned}
&Y = a + b_1X_1 \quad \text{(Linear model)},\\
&Y = a + b_1X_2 + b_2X_2^2 \quad \text{(Quadratic model)},\\
&Y = a + b_1X_3 + b_2X_3^2 + b_3X_3^3 \quad \text{(Cubic model)}.
\end{aligned}$$

In this context, Y represents the dependent variable, a represents the regression constant, b_i $(i = 1, 2, 3)$ is the regression coefficient and X_i $(i = 1, 2, 3)$ denotes the independent variable. The regression equation is constructed using the sample data. To assess the reliability and the predictive accuracy of the developed models, some supporting statistical parameters are employed, including the correlation coefficient (r), the coefficient of determination (r^2), significance F value $(Sig.\ F)$ and $F-$value. The correlation coefficient (r), ranging from -1 to $+1$, indicates both strength and the direction of the relationship between two variables X and Y. In general, $|r| \geq 0.7$ reflects a strong correlation, while $|r| \geq 0.5$ indicates moderate correlation.

Structural isomers are chemical compounds that share the same molecular formula but differ in the connectivity of their atoms. Octane isomers are chemical compounds with the molecular formula C_8H_{18} but vary in their structural configurations. These isomers are significant in the oil, gas and automotive industries, where they are used to improve fuel quality, enhance combustion efficiency and reduce harmful emissions. Consequently, octane isomers are commonly employed as standard reference compounds for evaluating gasoline performance.

In addition to their industrial relevance, octane isomers are used in the manufacture of solvents, plastics and detergents. From a scientific perspective, they serve as important model compounds in organic chemistry for studying reactions mechanisms and structure-property relationships. They are also utilized as reference fuels in aerospace engineering to analyze combustion characteristics and engine performance. Moreover, certain octane isomers have reported medical applications, including their use in anesthetic formulations and cancer-related research. Owing to their well defined structures and diverse physico-chemical properties, octane isomers are frequently used as test compounds for newly introduced graph invariants. In this study, octane isomers are employed to examine the relationship between the studied VDB vertex energy invariants and the eigenvector centrality measure.

In this section, we examine the relationship between eigenvector centrality measure ($\mathcal{X}_i$) and the various VDB vertex energies such as $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$, $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$, $\mathcal{F}\mathcal{E}_{\mathrm{G}}(v)$, $\mathcal{SO}\mathcal{E}_{\mathrm{G}}(v)$ and $\mathcal{ABC}\mathcal{E}_{\mathrm{G}}(v)$, which are derived from their respective VDB topological indices. The correlation is performed at the vertex level for octane isomers. Linear regression models have been employed to establish the relationship between eigenvector centrality measure and the various VDB vertex energies of octane isomers, thereby assessing the relevance of these parameters. The computed VDB vertex energy values and the corresponding eigenvector centrality measure values for each isomer are provided in Tables 8-10. Throughout the analysis, eigenvector centrality measure ($\mathcal{X}_i$) is taken as the independent variable X, while the VDB vertex energy invariants are considered as the dependent variable Y. The notation used to represent each isomer is provided in Table 6.

Regression models employed in the analysis and their corresponding statistical parameters are detailed in Tables 11-13. The associated correlation graphs have been provided in Figure 1 and 2. Figure 3 illustrates the heat map representation of the correlation coefficients obtained from the linear regression analysis between the VDB vertex energy invariants and the eigenvector centrality measure for each isomer. The standard values of $\mathcal{X}_i$ are taken from the article [43].

Octane isomer	**Notation**
n-octane	O1
2-methyl heptane	O2
3-methyl heptane	O3
4-methyl heptane	O4
3-ethyl hexane	O5
2, 2-dimethyl hexane	O6
2, 3-dimethyl hexane	O7
2, 4-dimethyl hexane	O8
2, 5-dimethyl hexane	O9
3, 3-dimethyl hexane	O10
3, 4-dimethyl hexane	O11
2-methyl 3-ethyl pentane	O12
3-methyl 3-ethyl pentane	O13
2, 2, 3-trimethyl pentane	O14
2, 2, 4-trimethyl pentane	O15
2, 3, 3-trimethyl pentane	O16
2, 3, 4-trimethyl pentane	O17
2, 2, 3, 3-tetramethyl butane	O18

Table 6. Notation used for denoting the octane isomers

Vertex energy invariant	**Notation**
Vertex energy	$\mathcal{E}_{\mathrm{G}}(v)$
First Zagreb vertex energy	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$
Second Zagreb vertex energy	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$
Forgotten vertex energy	$\mathcal{FE}_{\mathrm{G}}(v)$
Sombor vertex energy	$\mathcal{SOE}_{\mathrm{G}}(v)$
Atom-bond connectivity vertex energy	$\mathcal{ABCE}_{\mathrm{G}}(v)$

Table 7. Notation used for the studied VDB vertex energy invariants in correlation graphs

Isomer	**Parameter**	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
O1	$\mathcal{X}_i$	0.1612	0.303	0.4082	0.4642	0.4642	0.4082	0.303	0.1612
	$\mathcal{E}_{\mathrm{G}}(v)$	0.8620	1.3569	1.2529	1.2868	1.2868	1.2529	1.3569	0.8620
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.4382	4.6894	5.1187	5.1095	5.1095	5.1187	4.6894	2.4382
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.4442	4.0607	5.233	5.0727	5.0727	5.233	4.0607	1.4442
	$\mathcal{FE}_{\mathrm{G}}(v)$	3.8764	8.7149	10.3503	10.1803	10.1803	10.3503	8.7149	3.8764
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.8394	3.3963	3.6068	3.6174	3.6174	3.6068	3.3963	1.8394
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.6096	0.9595	0.886	0.9099	0.9099	0.886	0.9595	0.6096
O2	$\mathcal{X}_i$	0.2673	0.5211	0.4816	0.4179	0.3333	0.2319	0.1189	0.2673
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6259	1.6985	1.1414	1.3206	1.1830	1.3621	0.8050	0.6259
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.3797	7.3693	5.3293	5.1583	4.9546	4.7119	2.1962	2.3797
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5485	7.0460	6.4431	4.9300	5.2172	4.0522	1.2710	1.5485
	$\mathcal{FE}_{\mathrm{G}}(v)$	5.8277	18.8550	12.5764	10.1312	10.1335	8.7580	3.3790	5.8277
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9174	5.6337	3.7405	3.6647	3.4725	3.4134	1.6638	1.9174
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5236	1.3352	0.7898	0.9378	0.8329	0.9636	0.5669	0.5236
O3	$\mathcal{X}_i$	0.1927	0.3834	0.5698	0.4635	0.3521	0.2369	0.1191	0.2865
	$\mathcal{E}_{\mathrm{G}}(v)$	0.9111	1.3146	1.6426	1.2391	1.2772	1.3528	0.8737	0.7982
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.5600	5.0739	7.8111	5.4702	5.1523	4.6751	2.4859	2.7902
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.4903	5.2340	8.7291	6.0811	5.2004	4.0499	1.4913	1.5461
	$\mathcal{FE}_{\mathrm{G}}(v)$	4.0704	11.2680	20.4432	12.5332	10.3268	8.6878	4.0015	6.3530
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9351	3.6831	5.7876	3.8898	3.6363	3.3858	1.8758	2.2761
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.6506	0.9224	1.2368	0.8668	0.9078	0.9558	0.6201	0.6703
O4	$\mathcal{X}_i$	0.1443	0.2887	0.433	0.5774	0.433	0.2887	0.1443	0.2887
	$\mathcal{E}_{\mathrm{G}}(v)$	0.7702	1.3738	1.1036	1.6667	1.1036	1.3738	0.7702	0.6667
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.1020	4.7160	5.2915	7.7873	5.2915	4.7160	2.1020	2.4322
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.2372	3.9691	6.2832	8.5445	6.2832	3.9691	1.2372	1.4420
	$\mathcal{FE}_{\mathrm{G}}(v)$	3.2480	8.6423	12.5460	20.2634	12.5460	8.6423	3.2480	5.9600
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.5900	3.4183	3.7178	5.7828	3.7178	3.4183	1.5900	2.0039
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5394	0.9734	0.7670	1.2503	0.7670	0.9734	0.5394	0.5844
O5	$\mathcal{X}_i$	0.1899	0.3851	0.5914	0.4294	0.2796	0.1378	0.3851	0.1899
	$\mathcal{E}_{\mathrm{G}}(v)$	0.8907	1.3258	1.5782	1.2165	1.3632	0.8549	1.3258	0.8907
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.5111	5.0487	8.2274	5.4481	4.6960	2.4000	5.0487	2.5111
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5314	4.9328	10.1159	6.0275	4.0779	1.3634	4.9328	1.5314
	$\mathcal{FE}_{\mathrm{G}}(v)$	3.9653	11.0860	21.8953	12.5297	8.6576	3.7819	11.0860	3.9653
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.8837	3.6923	5.9283	3.8855	3.3944	1.8197	3.6923	1.8837
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.6299	0.9375	1.1160	0.8602	0.9640	0.6045	0.9375	0.6299
O6	$\mathcal{X}_i$	0.3019	0.6376	0.4409	0.2936	0.1792	0.0849	0.3019	0.3019
	$\mathcal{E}_{\mathrm{G}}(v)$	0.5370	1.9747	1.1962	1.2982	1.3492	0.8835	0.5370	0.5370
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.5674	10.4174	5.7979	5.2012	4.6560	2.5375	2.5674	2.5674
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.7676	10.3751	7.6146	5.1005	4.0793	1.5212	1.7676	1.7676
	$\mathcal{FE}_{\mathrm{G}}(v)$	8.5478	35.4134	15.6399	10.3799	8.6322	4.1221	8.5478	8.5478
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.1465	8.3577	4.1384	3.6798	3.3712	1.9117	2.1465	2.1465
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.4732	1.6462	0.8250	0.9244	0.9528	0.6269	0.4732	0.4732

Table 8. Values of $\mathcal{X}_i$ and the studied VDB vertex energy invariants for the isomers O1 – O6

Isomer	**Parameter**	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
O7	$\mathcal{X}_i$	0.2454	0.509	0.5651	0.3907	0.2454	0.1183	0.2454	0.2724
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6633	1.6703	1.6265	1.1282	1.3704	0.7844	0.6633	0.7406
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.4953	7.7761	8.2108	5.3263	4.7028	2.1688	2.4953	2.6330
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5216	9.1290	10.7086	6.0024	4.0464	1.2758	1.5216	1.3911
	$\mathcal{FE}_{\mathrm{G}}(v)$	5.9792	21.4228	22.9060	12.4304	8.6195	3.3735	5.9792	6.2572
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.0123	5.8526	5.9976	3.7593	3.4059	1.6354	2.0123	2.1808
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5517	1.2986	1.2004	0.7836	0.9709	0.5474	0.5517	0.6451
O8	$\mathcal{X}_i$	0.2188	0.4467	0.4747	0.5227	0.3367	0.1649	0.2188	0.256
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6123	1.7048	1.0471	1.6594	1.3115	0.9183	0.6123	0.6992
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.3318	7.3581	5.5816	7.8109	5.0657	2.5970	2.3318	2.4551
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5132	6.9557	7.3346	8.5961	5.3134	1.5048	1.5132	1.3822
	$\mathcal{FE}_{\mathrm{G}}(v)$	5.7406	18.6976	14.5307	20.2800	11.3050	4.1380	5.7406	5.7986
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.8811	5.6250	3.9128	5.7909	3.6759	1.9598	1.8811	2.0249
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5124	1.3395	0.6961	1.2481	0.9203	0.6549	0.5124	0.6013
O9	$\mathcal{X}_i$	0.2236	0.4472	0.4472	0.4472	0.4472	0.2236	0.2236	0.2236
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6472	1.6944	1.2472	1.2472	1.6944	0.6472	0.6472	0.6472
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.4627	7.3633	5.5447	5.5447	7.3633	2.4627	2.4627	2.4627
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5917	7.0845	6.3904	6.3904	7.0845	1.5917	1.5917	1.5917
	$\mathcal{FE}_{\mathrm{G}}(v)$	5.9607	18.8706	12.7938	12.7938	18.8706	5.9607	5.9607	5.9607
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9752	5.6289	3.9256	3.9256	5.6289	1.9752	1.9752	1.9752
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5366	1.3329	0.8747	0.8747	1.3329	0.5366	0.5366	0.5366
O10	$\mathcal{X}_i$	0.1755	0.3786	0.6409	0.4093	0.2417	0.1121	0.2972	0.2972
	$\mathcal{E}_{\mathrm{G}}(v)$	0.9348	1.2870	1.9450	1.0633	1.3800	0.7576	0.5760	0.5760
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.6550	5.3883	10.8488	5.5671	4.7400	2.0367	2.6259	2.6259
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5351	6.3618	12.4344	7.2451	3.9861	1.1781	1.5853	1.5853
	$\mathcal{FE}_{\mathrm{G}}(v)$	4.2832	14.2375	36.8669	15.3740	8.7153	3.0604	8.5968	8.5968
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.0036	3.9514	8.4796	3.9550	3.4354	1.5406	2.2358	2.2358
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.6689	0.8965	1.5517	0.7271	0.9794	0.5271	0.5246	0.5246
O11	$\mathcal{X}_i$	0.1601	0.3355	0.5428	0.5428	0.3355	0.1601	0.2591	0.2591
	$\mathcal{E}_{\mathrm{G}}(v)$	0.9062	1.3195	1.6135	1.6135	1.3195	0.9062	0.8266	0.8266
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.5340	5.0740	8.1971	8.1971	5.0740	2.5340	2.8733	2.8733
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.4638	5.0640	10.5119	10.5119	5.0640	1.4638	1.5434	1.5434
	$\mathcal{FE}_{\mathrm{G}}(v)$	3.9814	11.1922	22.8563	22.8563	11.1922	3.9814	6.5439	6.5439
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9142	3.6925	5.9970	5.9970	3.6925	1.9142	2.3583	2.3583
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.6467	0.9275	1.1954	1.1954	0.9275	0.6467	0.7000	0.7000
O12	$\mathcal{X}_i$	0.1601	0.3355	0.5428	0.5428	0.3355	0.1601	0.2591	0.2591
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6350	1.6801	1.4552	1.3401	0.8175	0.6350	1.3401	0.8175
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.4261	7.7368	8.5357	5.0658	2.2403	2.4261	5.0658	2.2403
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5977	8.7344	11.9905	4.6505	1.4248	1.5977	4.6505	1.4248
	$\mathcal{FE}_{\mathrm{G}}(v)$	5.9711	21.1825	24.3384	10.9812	3.4321	5.9711	10.9812	3.4321
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9563	5.8456	6.0487	3.7243	1.6665	1.9563	3.7243	1.6665
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5346	1.3064	0.9945	0.9513	0.5726	0.5346	0.9513	0.5726

Table 9. Values of $\mathcal{X}_i$ and the studied VDB vertex energy invariants for the isomers O7 – O12

Isomer	**Parameter**	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
O13	$\mathcal{X}_i$	0.1696	0.3713	0.6432	0.3713	0.1696	0.2938	0.3713	0.1696
	$\mathcal{E}_{\mathrm{G}}(v)$	0.9186	1.2966	1.8898	1.2966	0.9186	0.7559	1.2966	0.9186
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.6100	5.3549	11.2848	5.3549	2.6100	3.0499	5.3549	2.6100
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5982	5.8367	14.3047	5.8367	1.5982	1.5894	5.8367	1.5982
	$\mathcal{FE}_{\mathrm{G}}(v)$	4.2268	13.9743	38.3561	13.9743	4.2268	9.1138	13.9743	4.2268
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9637	3.9593	8.6031	3.9593	1.9637	2.6162	3.9593	1.9637
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.6574	0.9082	1.4357	0.9082	0.6574	0.6833	0.9082	0.6574
O14	$\mathcal{X}_i$	0.2729	0.6019	0.5092	0.2905	0.1317	0.2729	0.2729	0.2308
	$\mathcal{E}_{\mathrm{G}}(v)$	0.5469	1.9573	1.5881	1.3239	0.9022	0.5469	0.5469	0.8497
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.5936	10.8208	8.5717	5.0844	2.5084	2.5936	2.5936	2.9557
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.6813	13.1761	12.8934	4.7589	1.4802	1.6813	1.6813	1.4826
	$\mathcal{FE}_{\mathrm{G}}(v)$	8.5722	37.8325	26.1206	11.2079	3.9109	8.5722	8.5722	6.7077
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.1820	8.5268	6.2231	3.7086	1.8957	2.1820	2.1820	2.4294
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.4837	1.6128	1.1661	0.9311	0.6443	0.4837	0.4837	0.7178
O15	$\mathcal{X}_i$	0.2799	0.6015	0.4529	0.3717	0.1730	0.2799	0.2799	0.1730
	$\mathcal{E}_{\mathrm{G}}(v)$	0.5158	1.9816	0.9500	1.7107	0.5975	0.5158	0.5158	0.5975
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.4971	10.3993	5.7490	7.3584	2.2586	2.4971	2.4971	2.2586
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.7737	10.1985	8.6604	6.7831	1.5001	1.7737	1.7737	1.5001
	$\mathcal{FE}_{\mathrm{G}}(v)$	8.4968	35.2661	17.2153	18.5929	5.5766	8.4968	8.4968	5.5766
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.0961	8.3468	4.0282	5.6275	1.8288	2.0961	2.0961	1.8288
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.4604	1.6499	0.6075	1.3437	0.5025	0.4604	0.4604	0.5025
O16	$\mathcal{X}_i$	0.2115	0.4700	0.6210	0.3505	0.1578	0.2115	0.2795	0.2795
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6708	1.6540	1.9165	1.2917	0.9294	0.6708	0.6209	0.6209
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.5379	8.1190	11.2739	5.3760	2.6318	2.5379	2.7432	2.7432
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5524	11.0700	15.1832	5.8139	1.5690	1.5524	1.4865	1.4865
	$\mathcal{FE}_{\mathrm{G}}(v)$	6.1534	24.4855	39.3561	14.0536	4.2337	6.1534	8.6788	8.6788
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.0470	6.0807	8.6534	3.9618	1.9849	2.0470	2.3449	2.3449
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5589	1.2782	1.5095	0.9007	0.6659	0.5589	0.5572	0.5572
O17	$\mathcal{X}_i$	0.2176	0.4647	0.5573	0.4647	0.2176	0.2176	0.2610	0.2176
	$\mathcal{E}_{\mathrm{G}}(v)$	0.6586	1.6746	1.5776	1.6746	0.6586	0.6586	0.8628	0.6586
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.4766	7.7539	8.6062	7.7539	2.4766	2.4766	3.0049	2.4766
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5851	8.6988	12.5409	8.6988	1.5851	1.5851	1.4835	1.5851
	$\mathcal{FE}_{\mathrm{G}}(v)$	5.9684	21.1721	25.3518	21.1721	5.9684	5.9684	6.8814	5.9684
	$\mathcal{SOE}_{\mathrm{G}}(v)$	1.9970	5.8477	6.1935	5.8477	1.9970	1.9970	2.4863	1.9970
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.5491	1.3016	1.1434	1.3016	0.5491	0.5491	0.7366	0.5491
O18	$\mathcal{X}_i$	0.2454	0.5651	0.5651	0.2454	0.2454	0.2454	0.2454	0.2454
	$\mathcal{E}_{\mathrm{G}}(v)$	0.5547	1.9415	1.9415	0.5547	0.5547	0.5547	0.5547	0.5547
	$\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	2.6207	11.2167	11.2167	2.6207	2.6207	2.6207	2.6207	2.6207
	$\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	1.5119	16.6304	16.6304	1.5119	1.5119	1.5119	1.5119	1.5119
	$\mathcal{FE}_{\mathrm{G}}(v)$	8.6240	41.1504	41.1504	8.6240	8.6240	8.6240	8.6240	8.6240
	$\mathcal{SOE}_{\mathrm{G}}(v)$	2.2132	8.7227	8.7227	2.2132	2.2132	2.2132	2.2132	2.2132
	$\mathcal{ABCE}_{\mathrm{G}}(v)$	0.4899	1.5922	1.5922	0.4899	0.4899	0.4899	0.4899	0.4899

Table 10. Values of $\mathcal{X}_i$ and the studied VDB vertex energy invariants for the isomers O13 – O18

Isomer	**Parameter**	**Regression equation**	r^2	r	F**−value**	**Sig.**F
O1	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 1.2908X + 0.7584$	0.5968	0.7726	8.8824	0.0246
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 8.9298X + 1.3551$	0.8605	0.9276	37.0063	0.0009
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 12.5931X - 0.2554$	0.9186	0.9584	67.7280	0.0002
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 21.5565X + 1.0774$	0.9010	0.9492	54.6001	0.0003
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 5.8861X + 1.1482$	0.8389	0.9159	31.2333	0.0014
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 0.9127X + 0.5363$	0.5968	0.7726	8.8824	0.0246
O2	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 1.8279X + 0.4923$	0.4233	0.6506	4.4033	0.0807
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 11.3290X + 0.5723$	0.7027	0.8382	14.1791	0.0093
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 14.8244X - 0.8837$	0.7666	0.8756	19.7082	0.0044
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 31.9989X - 1.1208$	0.8135	0.9019	26.1681	0.0022
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 8.1440X + 0.4911$	0.7031	0.8385	14.2070	0.0093
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.3984X + 0.3478$	0.4682	0.6843	5.2833	0.0612
O3	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 1.5095X + 0.6848$	0.5919	0.7694	8.7030	0.0256
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 11.2726X + 0.83316$	0.8264	0.9091	28.5572	0.0018
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 16.3278X - 1.0869$	0.8489	0.9213	33.7033	0.0011
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 34.5617X - 1.5393$	0.8981	0.9477	52.8923	0.0003
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 8.0567X + 0.6862$	0.8424	0.9178	32.0697	0.0013
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.1425X + 0.4819$	0.6756	0.8219	12.4943	0.0123
O4	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 1.6561X + 0.5657$	0.4892	0.6994	5.7467	0.0535
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 12.3253X + 0.3020$	0.8595	0.9271	36.6983	0.0009
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 17.4930X - 1.5604$	0.9063	0.9520	58.0021	0.0003
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 37.2679X - 2.7162$	0.9584	0.9790	138.4018	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 8.7855X + 0.3017$	0.8678	0.9315	39.3805	0.0008
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.2537X + 0.3921$	0.5491	0.7410	7.3053	0.0354
O5	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 1.5867X + 0.6674$	0.8046	0.8970	24.7081	0.0025
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 12.7818X + 0.3512$	0.9577	0.9786	135.7100	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 19.1403X - 1.8782$	0.9673	0.9835	177.7549	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 39.4300X - 3.1357$	0.9639	0.9818	160.0764	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 8.9969X + 0.3618$	0.9567	0.9781	132.5103	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.1219X + 0.4719$	0.8046	0.8970	24.7081	0.0025
O6	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 1.7141X + 0.4945$	0.3063	0.5535	2.6494	0.1547
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 13.3327X + 0.3027$	0.6538	0.8086	11.3326	0.0151
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 16.2833X - 0.9246$	0.6749	0.8215	12.4532	0.0124
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 54.3191X - 4.7804$	0.8448	0.9191	32.6523	0.0012
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 10.8210X + 0.0490$	0.7018	0.8378	14.1231	0.0094
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.5889X + 0.2945$	0.4388	0.6624	4.6916	0.0735

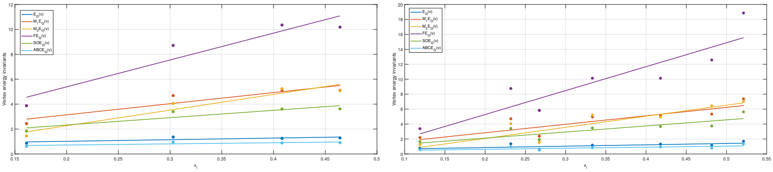
Table 11. Regression models used in the analysis and their corresponding statistical parameters for the isomers O1 − O6

Isomer	Parameter	Regression equation	r^2	r	$F-$value	Sig.F
O7	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 2.2780X + 0.3429$	0.6481	0.8050	11.0480	0.0159
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 15.1636X - 0.4364$	0.8739	0.9348	41.5864	0.0007
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 23.5849X - 3.1911$	0.8898	0.9433	48.4374	0.0004
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 47.9315X - 4.6570$	0.9467	0.9730	106.5706	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 10.9009X - 0.1744$	0.8931	0.9451	50.1494	0.0004
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.7044X + 0.2665$	0.7201	0.8486	15.4392	0.0077
O8	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 2.6334X + 0.2018$	0.6452	0.8033	10.9115	0.0163
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 16.0955X - 0.8686$	0.8855	0.9410	46.4051	0.0005
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 22.2975X - 3.0921$	0.9503	0.9748	114.7623	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 45.5639X - 4.2532$	0.9346	0.9667	85.7183	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 11.4066X - 0.4192$	0.8594	0.9270	36.6776	0.0009
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.8400X + 0.2036$	0.5893	0.7677	8.6108	0.0261
O9	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 3.6834X - 0.1764$	0.8715	0.9336	40.7040	0.0007
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 17.8503X - 1.5287$	0.9060	0.9518	57.8010	0.0003
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 23.0132X - 3.5541$	0.9910	0.9955	659.5300	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 44.1480X - 3.9108$	0.8407	0.9169	31.6663	0.0013
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 12.5314X - 0.8268$	0.8440	0.9187	32.4715	0.0013
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 2.5368X - 0.0306$	0.7540	0.8683	18.3895	0.0052
O10	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 2.0233X + 0.4194$	0.5024	0.7088	6.0576	0.0490
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 16.3238X - 0.6474$	0.8419	0.9176	31.9509	0.0013
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 22.5827X - 2.7164$	0.8527	0.9234	34.7264	0.0011
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 63.5691X - 7.8162$	0.9303	0.9645	80.0842	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 12.6645X - 0.5611$	0.8635	0.9293	37.9594	0.0008
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.6943X + 0.2594$	0.6232	0.7894	9.9238	0.0198
O11	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 2.0773X + 0.4927$	0.8396	0.9163	31.3958	0.0014
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 15.7192X - 0.4293$	0.9581	0.9788	137.2321	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 25.4322X - 3.6038$	0.9413	0.9702	96.2925	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 51.0329X - 5.4104$	0.9824	0.9912	334.8620	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 11.1605X - 0.1297$	0.9762	0.9880	246.399	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.5110X + 0.3773$	0.9609	0.9802	147.2617	0.0000
O12	$\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$	$Y = 2.3511X + 0.3276$	0.7506	0.8664	18.0560	0.0054
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$	$Y = 16.8472X - 0.9962$	0.9751	0.9875	234.8918	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$	$Y = 25.7461X - 3.8403$	0.9580	0.9788	136.9658	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{FE}_{\mathrm{G}}(v)$	$Y = 52.6244X - 6.2792$	0.9850	0.9925	392.9673	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_{\mathrm{G}}(v)$	$Y = 11.9771X - 0.5605$	0.9758	0.9878	241.7974	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$	$Y = 1.6582X + 0.2645$	0.7471	0.8643	17.7231	0.0056

Table 12. Regression models used in the analysis and their corresponding statistical parameters for the isomers O7 – O12

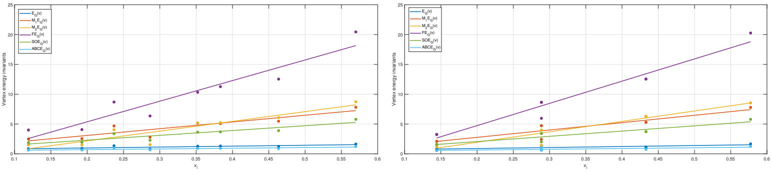
Isomer	**Parameter**	**Regression equation**	r^2	r	$F-$**value**	**Sig.**F
O13	$\mathcal{X}_i$ vs. $\mathcal{E}_G(v)$	$Y = 2.0806X + 0.4957$	0.8451	0.9193	32.7428	0.0012
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_G(v)$	$Y = 17.7737X - 0.9082$	0.9458	0.9725	104.6359	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_G(v)$	$Y = 26.3141X - 3.6447$	0.9305	0.9646	80.2975	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{FE}_G(v)$	$Y = 68.5751X - 9.1823$	0.9544	0.9769	125.6130	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_G(v)$	$Y = 13.4681X - 0.6858$	0.9535	0.9765	122.9967	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_G(v)$	$Y = 1.6005X + 0.3399$	0.9414	0.9702	96.3233	0.0001
O14	$\mathcal{X}_i$ vs. $\mathcal{E}_G(v)$	$Y = 2.8089X + 0.1259$	0.6532	0.8082	11.3027	0.0152
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_G(v)$	$Y = 19.9364X - 1.7212$	0.8953	0.9462	51.2985	0.0004
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_G(v)$	$Y = 31.6253X - 5.3558$	0.8893	0.9430	48.2085	0.0004
	$\mathcal{X}_i$ vs. $\mathcal{FE}_G(v)$	$Y = 74.7125X - 10.1839$	0.9600	0.9798	144.0186	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_G(v)$	$Y = 15.0848X - 1.2039$	0.9123	0.9552	62.4249	0.0002
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_G(v)$	$Y = 2.2603X + 0.0857$	0.7439	0.8625	17.4270	0.0058
O15	$\mathcal{X}_i$ vs. $\mathcal{E}_G(v)$	$Y = 3.3065X - 0.1564$	0.6569	0.8105	11.4878	0.0147
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_G(v)$	$Y = 19.5370X - 1.9389$	0.8443	0.9189	32.5328	0.0013
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_G(v)$	$Y = 23.7515X - 3.5088$	0.8767	0.9363	42.6632	0.0006
	$\mathcal{X}_i$ vs. $\mathcal{FE}_G(v)$	$Y = 66.6563X - 8.2969$	0.9163	0.9572	65.7037	0.0002
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_G(v)$	$Y = 14.9717X - 1.3943$	0.8296	0.9108	29.2158	0.0017
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_G(v)$	$Y = 2.5310X - 0.0779$	0.6061	0.7785	9.2305	0.0229
O16	$\mathcal{X}_i$ vs. $\mathcal{E}_G(v)$	$Y = 2.9650X + 0.0902$	0.7965	0.8925	23.4854	0.0029
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_G(v)$	$Y = 20.7912X - 1.9632$	0.9427	0.9709	98.6268	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_G(v)$	$Y = 33.4541X - 5.8301$	0.9285	0.9636	77.9055	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{FE}_G(v)$	$Y = 77.3451X - 10.9822$	0.9724	0.9861	211.6716	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_G(v)$	$Y = 15.5771X - 1.3431$	0.9575	0.9785	135.1254	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_G(v)$	$Y = 2.2837X + 0.0864$	0.8802	0.9382	44.0812	0.0006
O17	$\mathcal{X}_i$ vs. $\mathcal{E}_G(v)$	$Y = 3.3323X - 0.0375$	0.9318	0.9653	81.9752	0.0001
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_G(v)$	$Y = 19.7335X - 1.8299$	0.9866	0.9933	441.6000	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_G(v)$	$Y = 31.3036X - 5.5242$	0.9839	0.9919	366.1277	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{FE}_G(v)$	$Y = 59.9033X - 7.2977$	0.9929	0.9964	839.3463	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_G(v)$	$Y = 13.9073X - 1.0059$	0.9777	0.9888	263.5937	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_G(v)$	$Y = 2.3127X + 0.0781$	0.8830	0.9397	45.3020	0.0005
O18	$\mathcal{X}_i$ vs. $\mathcal{E}_G(v)$	$Y = 4.3377X - 0.5098$	1.0000	1.0000	1.12×10^{33}	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{M}_1\mathcal{E}_G(v)$	$Y = 26.8877X - 3.9775$	1.0000	1.0000	8.43×10^{32}	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{M}_2\mathcal{E}_G(v)$	$Y = 47.2896X - 10.0930$	1.0000	1.0000	1.51×10^{32}	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{FE}_G(v)$	$Y = 101.7404X - 16.3431$	1.0000	1.0000	7.36×10^{31}	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{SOE}_G(v)$	$Y = 20.3612X - 2.7834$	1.0000	1.0000	1.12×10^{32}	0.0000
	$\mathcal{X}_i$ vs. $\mathcal{ABCE}_G(v)$	$Y = 3.4478X - 0.3562$	1.0000	1.0000	1.69×10^{32}	0.0000

Table 13. Regression models used in the analysis and their corresponding statistical parameters for the isomers O13 – O18



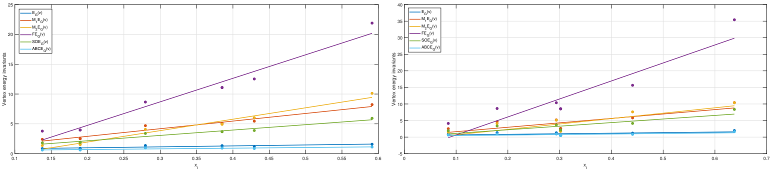
Correlation graph for O1

Correlation graph for O2



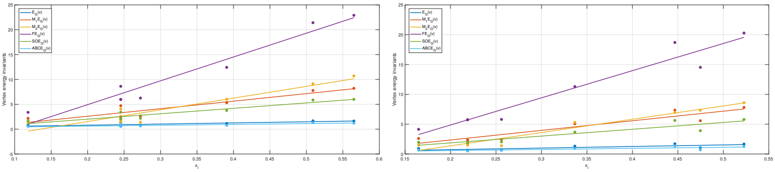
Correlation graph for O3

Correlation graph for O4



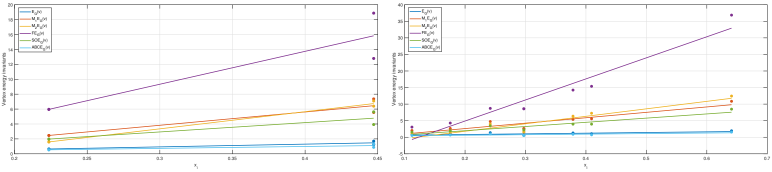
Correlation graph for O5

Correlation graph for O6



Correlation graph for O7

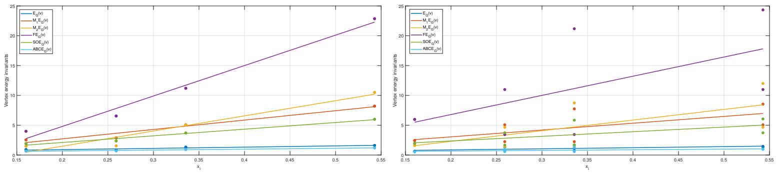
Correlation graph for O8



Correlation graph for O9

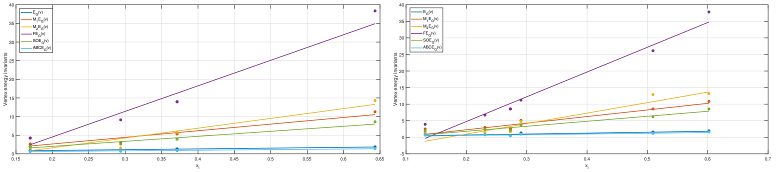
Correlation graph for O10

Figure 1. Correlation graphs for the isomer O1 – O10



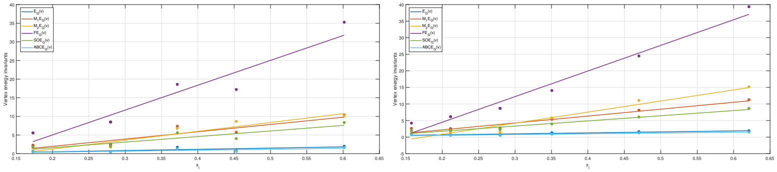
Correlation graph for O11

Correlation graph for O12



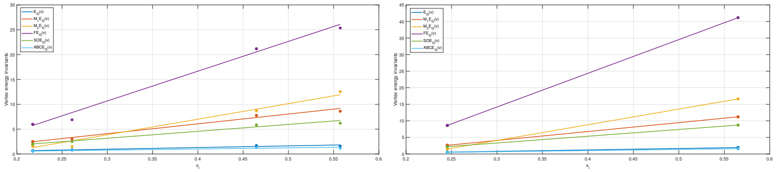
Correlation graph for O13

Correlation graph for O14



Correlation graph for O15

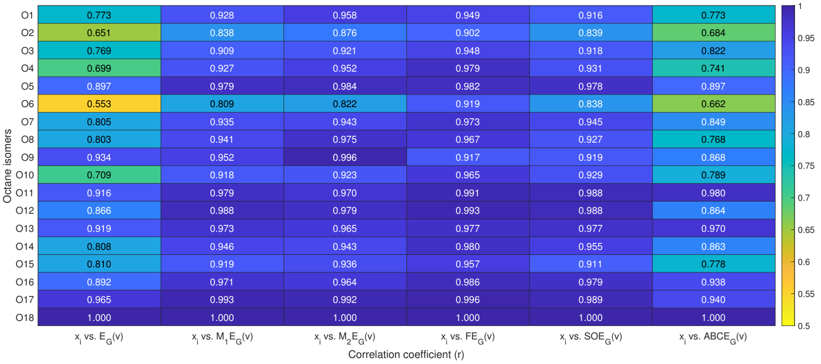
Correlation graph for O16



Correlation graph for O17

Correlation graph for O18

Figure 2. Correlation graphs for the isomer O11 – O18



Octane isomers	x_i vs. $E_G(v)$	x_i vs. $M_1E_G(v)$	x_i vs. $M_2E_G(v)$	x_i vs. $FE_G(v)$	x_i vs. $SOE_G(v)$	x_i vs. $ABCE_G(v)$
O1	0.773	0.928	0.958	0.949	0.916	0.773
O2	0.651	0.838	0.876	0.902	0.839	0.684
O3	0.769	0.909	0.921	0.948	0.918	0.822
O4	0.699	0.927	0.952	0.979	0.931	0.741
O5	0.897	0.979	0.984	0.982	0.978	0.897
O6	0.553	0.809	0.822	0.919	0.838	0.662
O7	0.805	0.935	0.943	0.973	0.945	0.849
O8	0.803	0.941	0.975	0.967	0.927	0.768
O9	0.934	0.952	0.996	0.917	0.919	0.868
O10	0.709	0.918	0.923	0.965	0.929	0.789
O11	0.916	0.979	0.970	0.991	0.988	0.980
O12	0.866	0.988	0.979	0.993	0.988	0.864
O13	0.919	0.973	0.965	0.977	0.977	0.970
O14	0.808	0.946	0.943	0.980	0.955	0.863
O15	0.810	0.919	0.936	0.957	0.911	0.778
O16	0.892	0.971	0.964	0.986	0.979	0.938
O17	0.965	0.993	0.992	0.996	0.989	0.940
O18	1.000	1.000	1.000	1.000	1.000	1.000

Figure 3. Heat map representation of correlation coefficients

5 Conclusion

Vertex energy and centrality measures are graph invariants that describe the contribution of the vertex energy of individual vertices to the total energy of a graph. Unlike global energy measures, they provide vertex-level information and allow the identification of structurally significant vertices. In this article, we have defined the general VDB vertex energy invariant by extending the notion of the energy of a vertex and have studied some particular VDB energy invariants, namely the first Zagreb vertex energy ($\mathcal{M}_1\mathcal{E}_{\mathrm{G}}(v)$), second Zagreb vertex energy ($\mathcal{M}_2\mathcal{E}_{\mathrm{G}}(v)$), forgotten vertex energy ($\mathcal{F}\mathcal{E}_{\mathrm{G}}(v)$), Sombor vertex energy ($\mathcal{SOE}_{\mathrm{G}}(v)$) and atom-bond connectivity vertex energy ($\mathcal{ABCE}_{\mathrm{G}}(v)$) and have computed their values for certain standard graphs. Subsequently, a vertex-level regression analysis has been performed between the eigenvector centrality measure ($\mathcal{X}_i$) and these VDB vertex energy invariants considering the 18 octane isomers. Linear regression models have been employed throughout the analysis. For the regression models corresponding to the isomers other than O2 and O6, it is observed that the correlation coefficient r is at least 0.7, $F-$value is at least 2.5 and the significant $F-$ value ($Sig.\, F$) is extremely low, approaching zero. These results indicate strong and statistically significant correlation between the considered VDB vertex energy invariants and the eigenvector centrality measure of these octane isomers. For the isomers O2 and O6, in the regression analysis of $\mathcal{X}_i$ vs. $\mathcal{E}_{\mathrm{G}}(v)$ and $\mathcal{X}_i$ vs. $\mathcal{ABCE}_{\mathrm{G}}(v)$, the correlation coefficient $r < 0.7$, indicating a moderate but statistically significant correlation between the variables. Overall, the VDB vertex energy invariants have shown a strong correlation with the eigenvector centrality measure, as evidenced by the regression analysis.

From a broader perspective, the present work deepens the understanding of how VDB vertex energy invariants capture structural asymmetry and branching characteristics in chemical isomers. Consequently, VDB vertex energy invariants serve as sensitive descriptors for identifying how atoms are structurally arranged in levels of importance or influence within the molecule. In recent years, atomic-level analysis has gained increasing importance in the biochemical sciences. The present work provides a foundation for the atomic-level characterization of chemical structures and consequently, for the application of vertex energy invariants in QSAR and QSPR studies. Moreover, the proposed approach can be extended to various graph operations, allowing the examination of changes in vertex energy under symmetric and asymmetric conditions. Additional classes of VDB vertex energy invariants can also be formulated and studied. Further, QSPR/QSAR studies can be conducted for special classes of chemical compounds using these VDB vertex energy invariants as molecular descriptors.

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