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Vertex-Degree-Based Energy for Selected Classes of Molecular Graphs

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Abstract

Vertex-degree-based matrices and their corresponding energies provide a unified framework that encompasses many matrices and energies induced by classical vertex-degree-based topological indices. This framework is motivated by the correlation between these indices and the structural and energetic properties of chemical compounds. Closed-form expressions for the energies induced by vertex-degree-based functions of a highly general four-parameter form are derived for several representative classes of graphs, including some graph products. This offers new insights into the spectral behaviour of molecular structures and expands the applicability of vertex-degree-based descriptors to a broader range of chemical and network systems, as well as QSAR/QSPR modelling.

1 Introduction

In the field of chemical graph theory, graph invariants are an excellent mathematical tool for studying the structural properties of different chemical compounds (see, for example, [1–3]). Among the most useful are the topological indices attached to an undirected simple graph $G = (V, E)$, defined by:

$$TI(G) = \sum_{v_iv_j \in E} \varphi(d_i, d_j), \tag{1}$$

where φ is an appropriately chosen function, and d_i is the degree of a vertex $v_i \in V$. These are referred to as *vertex-degree-based* (VDB) indices [4–6]. The matrix (usually referred to as the

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VDB matrix) induced by the VDB topological index $TI(G)$ is the square matrix of order $|V|$, whose element at position (i,j) is defined by:

$$\begin{cases} \varphi(d_i,d_j), & \text{if } v_iv_j \in E, \\ 0, & \text{if } v_iv_j \notin E, \\ 0, & \text{if } i=j. \end{cases}$$

This matrix structure was introduced as a natural extension of classical graph adjacency matrices, embedding degree-based information directly into edge weights.
The energy of a graph corresponding to a matrix derived from a topological index is defined as the sum of the absolute values of that matrix's eigenvalues.

The recently conceived *Sombor index* [7], defined by selecting $\varphi(x,y) = \sqrt{x^2+y^2}$ has attracted much attention. This VDB molecular structure descriptor is based on geometric considerations [7–10]. Some of its several noteworthy applications are [11–18]. The results of mathematical investigations into the Sombor index can be found in the review [19].
The Sombor matrix, the matrix associated with the Sombor index, was introduced in [7, 20], and has since been investigated by numerous authors, see, e.g., [20–28].

To obtain more effective and discriminative molecular descriptors, the function underlying the Sombor matrix, originally based on the Euclidean distance, has been further generalized and refined. As a result, several modified forms of the Sombor matrix have been introduced and analyzed, including the modified Sombor [3], the elliptic Sombor [29], Euler–Sombor [30], p-Sombor [31], and the diminished Sombor matrices [32]. These variants aim to capture additional structural nuances and enhance the sensitivity of Sombor-based indices to different molecular configurations.

Beyond these Sombor-driven formulations, further notable instances arise from alternative choices of the function φ. Well-known representatives include AG, GA, Gourava, Randić, Zagreb, and several related indices, whose original formulations and subsequent spectral investigations are concisely listed in Appendix A. Table 2 compiles the sources in which these indices were introduced, as well as key references analysing the associated VDB matrices and their energies, thereby offering a convenient overview of their presence and development in the existing literature.

Some compounds can be represented by graphs that arise as products of simpler component graphs [33]. Consequently, it is of interest to study how various graph invariants behave under these product operations and how they relate to the corresponding invariants of the factor graphs [34]. Therefore, analysing topological indices, the associated matrices and corresponding graph energies for certain graph products provides a deeper understanding of how molecular structure influences spectral and energetic properties.

Several studies have investigated topological indices for graph products, including [33, 35–37]. In many of the resulting formulas, the contributions of the individual factor graphs, as well as the interactions arising from the specific definition of the considered product, can be clearly identified. By contrast, when examining the energy associated with a graph product, the interdependence between the factors is deeply embedded in the structure of the corresponding matrix. Consequently, computing the energy is often challenging, and there is no clear direct analytical relationship between the energy of the product and the energies of its factors.

However, there are classes of graphs for which a direct relationship can be established between the VDB matrix and the adjacency matrix. In such cases, known spectral results describing the spectrum of the adjacency matrix of a product graph in terms of the spectra of its factors can be utilized to derive results for the corresponding energy of the product. These classes include regular and semiregular bipartite graphs. This makes it possible to compute the

VDB energy for a wide range of graphs that are relevant in practice, such as cycles, complete graphs, star graphs, complete bipartite graphs and various products derived from them.

Also, a broad and significant class of graphs exists for which such a direct connection does not hold. Numerous examples of graphs belonging to these classes demonstrate that no straightforward relationship can be established between the spectrum of a product graph's VDB matrix and the spectra of its factors. Alternative analytical or computational methods must therefore be employed to determine the corresponding spectrum and the associated energy for such products.

The present paper investigates a highly general form of VDB matrices for several selected graph families and their corresponding energies. Specifically, we study VDB matrices induced by functions φ of a highly general four-parameter form (defined by (3)), where appropriate parameter choices recover not only the classical Sombor matrix and its known modifications, but also numerous other matrices, as listed in Table 2.
This unified formulation enables the systematic introduction and analysis of new VDB indices, their corresponding matrices, and the associated spectral energies. Furthermore, examining continuous variations of one or more parameters within selected ranges allows us to analyse the influence and emergence of individual terms within the defining function in more detail, providing deeper insight into the structural and energetic behaviour of the resulting descriptors.

Let Φ denote the family of functions φ of the form (3). The general form of the VDB matrix corresponding to $\varphi \in \Phi$ will be called the Φ–VDB matrix, and the associated energy the Φ–VDB energy. We calculate the Φ–VDB energy for some graph families, including cycles of any order, complete graphs, star graphs, and certain graph products containing factors from these families, such as the closed fence graph, Hamming graphs, and their complements. Particular focus is given to the products of star and wheel graphs with K_2, as such structures are of notable interest in chemistry.
To obtain closed-form expressions, certain trigonometric sums are evaluated. The resulting formulas are particularly useful for numerical computations, as they enable fast and stable evaluation across wide parameter ranges.

It should be noted that the definition of the Φ–VDB matrix itself and most of the associated terms and results are largely independent of the traditional construction using vertex degrees. In fact, the same computational framework can be applied when the considered function depends on other vertex characteristics.
For example, in [38], a variant of the Sombor matrix was defined in which the vertex degree was replaced by the number of geodesic paths passing through that vertex. This quantity is known as the vertex stress. Similarly, multiplicative and additive variants of Szeged weights based on vertex partitions are used for matrix construction and further research in [39] and [40]. This extends the applicability of Φ–VDB matrices beyond purely degree-based formulations.
Although these concepts were initially introduced within the framework of mathematical chemistry, their scope extends to numerous other disciplines. Investigating graph invariants is important for various network-theoretical applications in fields such as the social sciences, communication networks, biological systems, and complex data structures [37].

2 Preliminaries

2.1 Some graphs and their spectra

Unless stated otherwise, the spectrum of a graph G refers to the spectrum of its adjacency matrix $\mathbf{A}(G)$. The spectra of cycles, complete graphs, and complete bipartite graphs are described in the following proposition.

Proposition 2.1 ([41], Lemma 2.1; [42], pages 8-9). *The spectrum of the adjacency matrix for the cyclic graph C_n, complete graph K_n, and complete bipartite graph $K_{p,q}$ are given by:*

$$
\begin{aligned}
SA_{C_n} &= \left\{ 2\cos\left(\frac{2\pi j}{n}\right) : j = 0, \ldots, n-1 \right\}, \\
SA_{K_n} &= \{n-1, -1\}, \ \textit{where } m(n-1) = 1 \textit{ and } m(-1) = n-1, \\
SA_{K_{p,q}} &= \{\sqrt{pq}, -\sqrt{pq}, 0\}, \ \textit{where } m(\sqrt{pq}) = m(-\sqrt{pq}) = 1 \textit{ and} \\
&\quad\ m(0) = p+q-2.
\end{aligned}
$$

Here, $m(\lambda)$ denotes the multiplicity of eigenvalue λ.

2.2 Graph products and their spectra

Theoretically, it is possible to define many products of two given graphs. Three of them are standard: these are the Cartesian product, the direct product, and the strong product of graphs. Here, we summarize their definitions and information about their spectra (see, for example, [42] or [43]).

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple finite graphs. In all cases, the vertex sets are the same and defined as $V = V_1 \times V_2$.

The Cartesian product of graphs G_1 and G_2, denoted by $G_1 \square G_2$, is a graph operation that produces a new graph $G_C = (V, E_C)$ such that there is an edge between $\mathbf{v}_1 = (v_{11}, v_{21})$ and $\mathbf{v}_2 = (v_{12}, v_{22})$ if and only if one of the following holds $v_{11} = v_{12} \wedge (v_{21}, v_{22}) \in E_2$ or $v_{21} = v_{22} \wedge (v_{11}, v_{12}) \in E_1$.

The direct (Kronecker) product of graphs G_1 and G_2, denoted by $G_1 \otimes G_2$ is a graph operation that produces a new graph $G_K = (V, E_K)$ such that there is an edge between $\mathbf{v}_1 = (v_{11}, v_{21})$ and $\mathbf{v}_2 = (v_{12}, v_{22})$ if and only if $(v_{11}, v_{12}) \in E_1 \wedge (v_{21}, v_{22}) \in E_2$.

The strong product of two graphs is a graph operation that combines elements of both the Cartesian product and the direct product. The strong product of graphs G_1 and G_2, denoted by $G_1 \boxtimes G_2$ is a graph operation that produces a new graph $G_S = (V, E_S)$ such that $E_S = E_C \cup E_K$.

The spectra of graphs created using the introduced products are completely determined by the spectra of factors G_1 and G_2, as nicely summarized in [44, Table 4].

Also, by definition, it is easy to conclude that the regularity of graphs is preserved when applying these graph products (see, for example, [42, 43]), i.e. the Cartesian, direct and strong products of two regular graphs are also regular graphs. In Table 1, eigenvalues of the adjacency matrix for products under consideration are presented. Also, the degree of regularity is presented in the case of a regular factor.

Graph	Eigenvalues of adjacency matrix	Regularity r
G_1	λ_i	r_1
G_2	μ_j	r_2
$G_1 \square G_2$	$\lambda_i + \mu_j$	$r_1 + r_2$
$G_1 \otimes G_2$	$\lambda_i \mu_j$	$r_1 r_2$
$G_1 \boxtimes G_2$	$\lambda_i + \mu_j + \lambda_i \mu_j$	$r_1 r_2 + r_1 + r_2$

Table 1: Eigenvalues and regularity of graph products.

2.3 Evaluation of some trigonometric sums

In order to derive different $\Phi-$VDB energies for selected graphs and their products, we will use some trigonometric sums (determined by selecting specific values of parameters l and m), given in the following lemma. The proof of the lemma is given in Section 4.

Lemma 2.2. *Let* $A_n(l,m)=\sum_{j=0}^{n-1}\left|l\cos\frac{2\pi j}{n}+m\right|$, *then*

$$A_n(l,m)=\begin{cases} n\,|m|\,, & \textit{for}\ \ |m|\geq l,\\ m\,(4t+2-n)+2l\frac{\sin\left(\left(t+\frac{1}{2}\right)\frac{2\pi}{n}\right)}{\sin\left(\frac{\pi}{n}\right)}, & \textit{for}\ \ |m|<l. \end{cases} \tag{2}$$

where $t=\lfloor\frac{n}{2\pi}\arccos\left(-\frac{m}{l}\right)\rfloor$.

3 Results

3.1 $\Phi-$VDB matrix and its energy

Motivated by the existence of multiple variants of VDB matrices in the literature, especially the Sombor matrix and its modifications, we introduce a $\Phi-$VDB matrix defined by a parametric function of vertex degrees. Specifically, for real parameters $\alpha,\beta,\gamma,\delta$ let $\varphi^{\alpha,\beta,\gamma,\delta}$ be a function given by:

$$\varphi^{\alpha,\beta,\gamma,\delta}(x,y)=(x^\alpha+y^\alpha+\delta xy)^\beta(x+y)^\gamma. \tag{3}$$

Denote by Φ a family of such functions. Then a $\Phi-$VDB matrix $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$ is such that its (i,j)-entry is given by:

$$\begin{cases} \varphi^{\alpha,\beta,\gamma,\delta}(d_i,d_j), & \text{if}\ \ v_iv_j\in E,\\ 0, & \text{if}\ \ v_iv_j\notin E,\\ 0, & \text{if}\ \ i=j. \end{cases} \tag{4}$$

This formulation provides a unified framework that generalizes several known VDB matrices. For example, by choosing suitable values for α,β,γ, and δ, one recovers the classical Sombor matrix, the modified Sombor matrix, the elliptic Sombor matrix, as well as many other VDB matrices induced by classical topological indices, as listed in Table 2.

Similarly, we define the $\Phi-$VDB energy corresponding to the matrix $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$ as the sum of the absolute values of its eigenvalues

$$E^{\alpha,\beta,\gamma,\delta}(G)=\sum_{j=1}^{n}|\eta_j|, \tag{5}$$

where η_j are the eigenvalues of $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$. Note that, for an undirected simple graph G, the matrix $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$ is symmetric real, so all its eigenvalues are real.

3.2 $\Phi-$VDB energy for bipartite complete graphs

The simplest bipartite complete graph is the star graph $S_n=K_{n-1,1}$. All edges in S_n are between the central vertex of degree $n-1$ and the vertices of degree 1. Thus, all non-zero entries of the $\Phi-$VDB matrix are equal to $n^\gamma((n-1)^\alpha+1+\delta(n-1))^\beta$ and consequently,

$$\mathbf{A}^{\alpha,\beta,\gamma,\delta}(S_n)=n^\gamma((n-1)^\alpha+1+\delta(n-1))^\beta\mathbf{A}(S_n).$$

The obtained property, combined with the known spectra of the adjacency matrix $\mathbf{A}(S_n)$ for the star graph given in Proposition 2.1 (since $S_n = K_{n-1,1}$), implies the following proposition.

Proposition 3.1. *The spectrum of the* $\Phi-$*VDB matrix for the star graph* S_n *is given by* $S_{S_n} = \left\{s\sqrt{n-1}, -s\sqrt{n-1}, 0\right\}$, *where* $s = n^{\gamma}((n-1)^{\alpha} + 1 + \delta(n-1))^{\beta}$ *and* $m(s\sqrt{n-1}) = m(-s\sqrt{n-1}) = 1$ *and* $m(0) = n-2$, *while its* $\Phi-$*VDB energy is equal to*

$$E^{\alpha,\beta,\gamma,\delta}_{S_n} = 2s\sqrt{n-1}.$$

Analogous results can be derived for any bipartite complete graph $K_{p,q}$, since all the edges are between q and p degree vertices. Thus,

$$\mathbf{A}^{\alpha,\beta,\gamma,\delta}(K_{p,q}) = k(p,q)\mathbf{A}(K_{p,q}), \tag{6}$$

where $k(p,q) = (p^{\alpha} + q^{\alpha} + \delta pq)^{\beta}(p+q)^{\gamma}$, and the following proposition holds true.

Proposition 3.2. *The spectrum of the* $\Phi-$*VDB matrix for the complete bipartite graph* $K_{p,q}$ *is given by* $S_{K_{p,q}} = \left\{k(p,q)\sqrt{pq}, -k(p,q)\sqrt{pq}, 0\right\}$, *where* $m(k(p,q)\sqrt{pq}) = m(-k(p,q)\sqrt{pq}) = 1$ *and* $m(0) = p+q-2$, *while its* $\Phi-$*VDB energy is equal to*

$$E^{\alpha,\beta,\gamma,\delta}_{K_{p,q}} = 2k(p,q)\sqrt{pq}.$$

Note that the relation between the Φ–VDB matrix and the adjacency matrix observed for complete bipartite graphs remains valid for all semiregular bipartite graphs. These are graphs such that each vertex in the same partition has the same degree. Namely, for bipartite graph $G_{r_1,r_2} = (V_1 \cup V_2, E)$, such that each vertex in V_1 has degree r_1 and each vertex in V_2 has degree r_2, all non-zero entries of the $\Phi-$VDB matrix are equal to $(r_1^{\alpha} + r_2^{\alpha} + \delta r_1 r_2)^{\beta}(r_1+r_2)^{\gamma}$ and consequently,

$$\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G_{r_1,r_2}) = k(r_1,r_2)\mathbf{A}(G_{r_1,r_2}). \tag{7}$$

This implies that the spectrum of the $\Phi-$VDB matrix and the corresponding energy can be determined from its adjacency spectrum.

Similarly, the obtained relation remains valid for all regular graphs. The next subsection summarizes the results for some important regular graphs.

3.3 $\Phi-$VDB energy for some regular graphs

For r-regular graph G, the relation between its adjacency matrix $\mathbf{A}(G)$ and the $\Phi-$VDB matrix $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$ is given by

$$\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G) = a(r)\mathbf{A}(G), \tag{8}$$

where,

$$a(r) = k(r,r) = (2r^{\alpha} + \delta r^2)^{\beta}(2r)^{\gamma}. \tag{9}$$

Due to this property, the eigenvalues of $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$ and $\mathbf{A}(G)$ are also related, i.e. $\eta_j = a(r)\lambda_j$, where η_j are the eigenvalues of $\mathbf{A}^{\alpha,\beta,\gamma,\delta}(G)$, and λ_j are the eigenvalues of $\mathbf{A}(G)$.
In the special case of some important regular graphs, Proposition 2.1 implies the following result.

Proposition 3.3. *The spectrum of the* $\Phi-$*VDB matrix* $\mathbf{A}^{\alpha,\beta,\gamma,\delta}$ *for the cyclic graph* C_n *and the complete graph* K_n *are given by:*

$$S_{C_n} = \left\{2b\cos\left(\frac{2\pi j}{n}\right) : j = 0, \dots, n-1\right\},$$

$$S_{K_n} = \quad \{(n-1)c, -c\}, \text{ where } m(cn-c) = 1 \text{ and } m(-c) = n-1,$$

where $b = a(2) = 4^\gamma(2^{\alpha+1}+4\delta)^\beta$ *and* $c = a(n-1) = (2n-2)^\gamma(2(n-1)^\alpha + \delta(n-1)^2)^\beta$.

Using the obtained eigenvalues, it is possible to deduce expressions for the corresponding energies. In the proofs, we will use the following lemma, which directly follows from Lemma 2.2, for $l = 1$ and $m = 0$.

Lemma 3.4. *Let* $A_n = A_n(1,0) = \sum_{j=0}^{n-1} \left|\cos \frac{2\pi j}{n}\right|$, *for* $n \geq 1$, *then*

$$A_n = \begin{cases} 2\cot\frac{\pi}{n}, & n \equiv 0 \pmod 4, \\ \csc\frac{\pi}{2n}, & n \equiv 1 \pmod 2, \\ 2\csc\frac{\pi}{n}, & n \equiv 2 \pmod 4. \end{cases} \tag{10}$$

Theorem 3.5. *The* $\Phi-$*VDB energy for the cyclic graph* C_n *and the complete graph* K_n *is given by*

$$\begin{aligned} E_{C_n}^{\alpha,\beta,\gamma,\delta} &= 2bA_n, \\ E_{K_n}^{\alpha,\beta,\gamma,\delta} &= 2c(n-1), \end{aligned}$$

where $b = 4^\gamma(2^{\alpha+1}+4\delta)^\beta$ *and* $c = (2n-2)^\gamma(2(n-1)^\alpha+\delta(n-1)^2)^\beta$.

Proof. The proof easily follows from the definition (5), using spectra given in Proposition 3.3 and expression given in Lemma 3.4. ■

Energies that correspond to the indices tabulated in Table 2 are special cases of energy defined by (5), and their precise values for selected graphs are tabulated in Table 3. We give results for cyclic C_n and complete K_n graphs for $n \geq 3$, star graph S_n, $n \geq 2$ and complete bipartite graph $K_{p,q}$, for $p \geq 1$ and $q \geq 1$.

3.4 $\Phi-$VDB energy for some graph operations of regular graphs

In order to derive closed formulas for $\Phi-$VDB energy for some graph products, we will use the following lemmas, that directly follows from Lemma 2.2.

Lemma 3.6. *Let* $B_n = A_n(2,-1) = \sum_{j=0}^{n-1} \left|2\cos\frac{2\pi j}{n} - 1\right|$, *for* $n \geq 2$, *then*

$$B_n = \begin{cases} \frac{n}{3} + 2\sqrt{3}\cot\frac{\pi}{n}, & n \equiv 0 \pmod 6, \\ \frac{n-4}{3} + 4\sin\frac{(n+2)\pi}{3n}\csc\frac{\pi}{n}, & n \equiv 1 \pmod 6, \\ \frac{n-2}{3} + 4\cos\frac{(n-2)\pi}{6n}\csc\frac{\pi}{n}, & n \equiv 2 \pmod 6, \\ \frac{n}{3} + 2\sqrt{3}\csc\frac{\pi}{n}, & n \equiv 3 \pmod 6, \\ \frac{n+2}{3} + 4\cos\frac{(n+2)\pi}{6n}\csc\frac{\pi}{n}, & n \equiv 4 \pmod 6, \\ \frac{n+4}{3} + 4\sin\frac{(n-2)\pi}{3n}\csc\frac{\pi}{n}, & n \equiv 5 \pmod 6. \end{cases} \tag{11}$$

Lemma 3.7. *Let* $D_n = B_n + A_n(2,1) = \sum_{j=0}^{n-1} \left(\left|2\cos\frac{2\pi j}{n} - 1\right| + \left|2\cos\frac{2\pi j}{n} + 1\right|\right)$, *for* $n \geq 1$, *then*

$$D_n = \begin{cases} \frac{2n}{3} + 4\sqrt{3}\cot\frac{\pi}{n}, & n \equiv 0 \pmod 6, \\ \frac{2(n-1)}{3} + 4\sin\frac{(2n+1)\pi}{6n}\csc\frac{\pi}{2n}, & n \equiv 1 \pmod 6, \\ \frac{2(n-2)}{3} + 8\cos\frac{(n-2)\pi}{6n}\csc\frac{\pi}{n}, & n \equiv 2 \pmod 6, \\ \frac{2n}{3} + 2\sqrt{3}\left(\csc\frac{\pi}{n} + \cot\frac{\pi}{n}\right), & n \equiv 3 \pmod 6, \\ \frac{2(n+2)}{3} + 8\cos\frac{(n+2)\pi}{6n}\csc\frac{\pi}{n}, & n \equiv 4 \pmod 6, \\ \frac{2(n+1)}{3} + 4\sin\frac{(2n-1)\pi}{6n}\csc\frac{\pi}{2n}, & n \equiv 5 \pmod 6. \end{cases} \tag{12}$$

3.4.1 The Cartesian product $G_1 \Box G_2$

$\Phi-$VDB energy for some Cartesian products of regular graphs is calculated in the following propositions.

Proposition 3.8. *For Hamming graph $G = H(2;p,q) = K_p \Box K_q$, for $p \geq 2$ and $q \geq 2$,*

$$E^{\alpha,\beta,\gamma,\delta}(G) = 2^{\gamma+2}(p+q-2)^{\gamma}(2(p+q-2)^{\alpha} + \delta(p+q-2)^2)^{\beta}(p-1)(q-1).$$

Proof. The spectrum of the complete graph K_p consists of the value $p-1$ with multiplicity 1 and the value -1 with multiplicity $p-1$. Similarly holds true for K_q. Using the property of eigenvalues of the Cartesian product follows that the spectrum of G contains the value $p+q-2$ (with multiplicity 1), the value $p-2$ with multiplicity $q-1$, $q-2$ with multiplicity $p-1$, and the value -2 with multiplicity $(p-1)(q-1)$. Thus, the sum of absolute values of eigenvalues of G is given by $4(p-1)(q-1)$. Since K_p is $(p-1)-$regular, and K_q iz $(q-1)-$regular, it follows that G is $(p+q-2)-$regular, thus

$$E^{\alpha,\beta,\gamma,\delta}(G) = 4a(p+q-2)(p-1)(q-1),$$

where $a(p+q-2)$ is defined by (9), which implies the result. ■

Proposition 3.9. *Let $G = K_2 \Box C_n$ for $n \geq 3$, then*

$$E^{\alpha,\beta,\gamma,\delta}(G) = 6^{\gamma}\left(2 \cdot 3^{\alpha} + 9\delta\right)^{\beta} D_n.$$

Proof. The spectrum of the complete graph K_2 consists of the eigenvalues -1 and 1, each with multiplicity 1, while the spectrum of the cycle graph C_n consists of eigenvalues $2\cos\frac{2\pi j}{n}$ for $j = 0,\ldots,n-1$. Therefore, the spectrum of the Cartesian product $G = K_2 \Box C_n$ consists of eigenvalues $1+2\cos\frac{2\pi j}{n}$ and $-1+2\cos\frac{2\pi j}{n}$, for $j = 0,\ldots,n-1$. The sum of absolute values of these eigenvalues is the sum D_n from Lemma 3.7. Since K_2 is $1-$regular and C_n is $2-$regular, it follows that G is $3-$regular. Thus

$$E^{\alpha,\beta,\gamma,\delta}(G) = a(3)D_n,$$

which gives the desired result. ■

Proposition 3.10. *Let $G = K_p \Box C_n$ for $p \geq 3$ and $n \geq 3$, then*

$$E^{\alpha,\beta,\gamma,\delta}(G) = (p-1)\left(2(p+1)\right)^{\gamma}\left(2(p+1)^{\alpha} + \delta(p+1)^2\right)^{\beta}(n+B_n).$$

Proof. The spectrum of the complete graph K_p and the spectrum of the cycle graph C_n implies that the spectrum of the Cartesian product G consists of values $p-1+2\cos\frac{2\pi j}{n}$ with multiplicity 1 and $-1+2\cos\frac{2\pi j}{n}$ with multiplicity $p-1$, for $j = 0,\ldots,n-1$. Thus, the sum of absolute values of the eigenvalues is given by:

$$\sum_{j=0}^{n-1}\left|p-1+2\cos\frac{2\pi j}{n}\right| + (p-1)\sum_{j=0}^{n-1}\left|-1+2\cos\frac{2\pi j}{n}\right|.$$

For $p \geq 3$, the term $p-1+2\cos\frac{2\pi j}{n}$ is non-negative for all j, and therefore the first sum simplifies to $n(p-1)$, since $\sum_{j=0}^{n-1}\cos\frac{2\pi j}{n} = 0$. Since K_p is $(p-1)-$regular and C_n is $2-$regular, if follows that G is $(p+1)-$regular. Hence,

$$E^{\alpha,\beta,\gamma,\delta}(G) = (p-1)a(p+1)(n+B_n),$$

where $a(p+1)$ is given by (9) and B_n is defined in Lemma 3.6. This completes the proof. ■

3.4.2 The direct product $G_1 \otimes G_2$

The following propositions can be proved using the procedure described in the proofs of the previous subsection. There, we combine the properties of the directed product given in Table 1, i.e., the form of its eigenvalues and the corresponding degree of regularity.

Proposition 3.11. *Let $G = K_p \otimes K_q$ for $p \geq 2$ and $q \geq 2$, then*

$$E^{\alpha,\beta,\gamma,\delta}(G) = 2^{\gamma+2}\left((p-1)(q-1)\right)^{\gamma+2\beta+1}\left(2\left((p-1)(q-1)\right)^{\alpha-2}+\delta\right)^{\beta}.$$

Proposition 3.12. *Let $G = K_p \otimes C_n$ for $p \geq 2$ and $n \geq 3$, then*

$$E^{\alpha,\beta,\gamma,\delta}(G) = 2^{2\gamma+2}(p-1)^{\gamma+1}\left(2^{\alpha+1}(p-1)^{\alpha}+4\delta(p-1)^2\right)^{\beta}A_n.$$

Results obtained in Propositions 3.8 and 3.11 do not contain any trigonometric sum, thus explicit expressions for selected $\Phi-$VDB energies associated to indices listed in Table 2 are quite simple, and they are tabulated in Table 4.

3.4.3 The strong product $G_1 \boxtimes G_2$

The analogous procedure, as in previous subsections, may yield the expression for the $\Phi-$VDB energy for $K_p \boxtimes K_q$. However, since, by definition, $K_p \boxtimes K_q = K_{pq}$, the result directly follows from Theorem 3.5

$$E^{\alpha,\beta,\gamma,\delta}(K_p \boxtimes K_q) = 2^{\gamma+1}(pq-1)^{\gamma+1}\left(2(pq-1)^{\alpha}+\delta(pq-1)^2\right)^{\beta}.$$

Proposition 3.13. *Let $G = K_2 \boxtimes C_n$ for $n \geq 3$, then*

$$E^{\alpha,\beta,\gamma,\delta}(K_2 \boxtimes C_n) = 10^{\gamma}(2\cdot 5^{\alpha}+25\delta)^{\beta}\left(4t+2+8\sin\left(\frac{2t+1}{n}\pi\right)\csc\left(\frac{\pi}{n}\right)\right),$$

where $t = \lfloor \frac{n}{2}\left(1-\frac{1}{\pi}\arccos\frac{1}{4}\right)\rfloor$.

Proof. Each vertex in G has degree 5, and Proposition 2.1 and the results given in Table 1 imply that its spectra consists of values $1+4\cos\frac{2\pi j}{n}$, $j = 0,\ldots,n-1$, with multiplicity 1, and the value -1 with multiplicity n. Thus

$$E^{\alpha,\beta,\gamma,\delta}(K_2 \boxtimes C_n) = a(5)\left(n+\sum_{j=0}^{n-1}\left|1+4\cos\frac{2\pi j}{n}\right|\right) = 10^{\gamma}(2\cdot 5^{\alpha}+25\delta)^{\beta}\left(n+A_n(4,1)\right),$$

and, since

$$A_n(4,1) \quad = \quad 4t-n+2+8\frac{\sin\left(\frac{2t+1}{n}\pi\right)}{\sin\left(\frac{\pi}{n}\right)},$$

where $t = \lfloor \frac{n}{2}\left(1-\frac{1}{\pi}\arccos\frac{1}{4}\right)\rfloor$, the proof is completed. ∎

3.5 $\Phi-$VDB energy for some graph operations of non-regular graphs

The $\Phi-$VDB energy expressions for several graph products, derived in the previous subsection, are established based on the relationship between adjacency and $\Phi-$VDB matrices implied by the regularity of the factor graphs, together with the spectral properties summarized in Table 1. In contrast, for non-regular graphs, the vertex-degree metric is inherently incorporated into the definition of the $\Phi-$VDB matrix, and consequently, straightforward eigenvalue relations no longer apply. In the sequel, we establish several formulas for the $\Phi-$VDB energy derived from block decompositions of the $\Phi-$VDB matrix induced by appropriate vertex enumerations.

Theorem 3.14. *Let $B_n = K_2\Box S_n$ for $n \geq 3$ be a n-book graph, then*

$$\begin{aligned} E^{\alpha,\beta,\gamma,\delta}(K_2\Box S_n) &= 2(n-2)B \\ &+ \left|B + C + \sqrt{(B-C)^2 + 4(n-1)A^2}\right| \\ &+ \left|B + C - \sqrt{(B-C)^2 + 4(n-1)A^2}\right|, \end{aligned}$$

where $A = \varphi^{\alpha,\beta,\gamma,\delta}(2,n)$, $B = \varphi^{\alpha,\beta,\gamma,\delta}(2,2)$, and $C = \varphi^{\alpha,\beta,\gamma,\delta}(n,n)$, with $\varphi^{\alpha,\beta,\gamma,\delta}$ defined by (3).

Proof. For simplicity, instead of the standard pair representation of vertices, we use a labeling that separates the vertices into two partitions, each associated with one copy of the star graph in the product. Denote by $v_1, v_2 \ldots, v_n$ vertices in the first copy of the star graph, with v_1 as the central point, and by $v_1', v_2', \ldots, v_n'$ corresponding vertices in the second copy. Thus, the adjacency, and consequently, the $\Phi-$VDB matrix can be written as a block matrix, where blocks correspond to the described vertex partition. It follows that

$$\mathbf{A}^{\alpha,\beta,\gamma,\delta}(K_2\Box S_n) = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{pmatrix},$$

where,

$$\mathbf{A} = \begin{pmatrix} 0 & A & A & \cdots & A \\ A & 0 & 0 & \cdots & 0 \\ A & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A & 0 & 0 & \cdots & 0 \end{pmatrix}_{n\times n} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} C & 0 & 0 & \cdots & 0 \\ 0 & B & 0 & \cdots & 0 \\ 0 & 0 & B & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & B \end{pmatrix}_{n\times n}.$$

Here, we use the fact that the star central vertices in the graph B_n are of degree n, while all other vertices are of degree 2. The structure of the obtained block matrix enables us to conclude that it is similar to $diag(\mathbf{A}+\mathbf{B}, \mathbf{A}-\mathbf{B})$, i.e.

$$P^T\mathbf{A}^{\alpha,\beta,\gamma,\delta}(K_2\Box S_n)P = diag(\mathbf{A}+\mathbf{B}, \mathbf{A}-\mathbf{B}),$$

where $P = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{-I} \end{pmatrix}$. Thus, the spectrum of the $\Phi-$VDB matrix consists of the spectra of $\mathbf{A}+\mathbf{B}$ and $\mathbf{A}-\mathbf{B}$.

The characteristic polynomial for $\mathbf{A}+\mathbf{B}$ can be easily obtained from the following property of the determinant of a block matrix consisting of four matrices $\mathbf{A}_j$, $j = 1,2,3,4$

$$\det\left(\begin{pmatrix} \mathbf{A}_1 & \mathbf{A}_2 \\ \mathbf{A}_3 & \mathbf{A}_4 \end{pmatrix}\right) = \det\left(\mathbf{A}_1 - \mathbf{A}_2\mathbf{A}_4^{-1}\mathbf{A}_3\right)\det(\mathbf{A}_4). \tag{13}$$

Taking single value matrix for $\mathbf{A}_1$, we deduce that

$$\begin{aligned} P_{\mathbf{A}+\mathbf{B}}(\lambda) &= det(\mathbf{A}+\mathbf{B}-\lambda\mathbf{I}_n) = \begin{vmatrix} C-\lambda & A & A & \cdots & A \\ A & B-\lambda & 0 & \cdots & 0 \\ A & 0 & B-\lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A & 0 & 0 & \cdots & B-\lambda \end{vmatrix} \\ &= \left(C-\lambda-\frac{(n-1)A^2}{B-\lambda}\right) det((B-\lambda)\mathbf{I}_{n-1}) \\ &= (\lambda^2-(B+C)\lambda+BC-(n-1)A^2)(B-\lambda)^{n-2}. \end{aligned}$$

Thus, the spectrum of $\mathbf{A}+\mathbf{B}$ consists of the value B with multiplicity $n-2$, and values $(B+C\pm\sqrt{(B-C)^2+4(n-1)A^2})/2$, with multiplicity 1.
An analogous procedure can be used to determine the spectrum of $\mathbf{A}-\mathbf{B}$. Since

$$\begin{aligned} P_{\mathbf{A}-\mathbf{B}}(\lambda) &= det(\mathbf{A}-\mathbf{B}-\lambda\mathbf{I}_n) \\ &= (\lambda^2+(B+C)\lambda+BC-(n-1)A^2)(-B-\lambda)^{n-2}, \end{aligned}$$

its spectrum consists of values $(-B-C\pm\sqrt{(B-C)^2+4(n-1)A^2})/2$, with multiplicity 1 and the value $-B$ with multiplicity $n-2$.
All the given facts, combined with a suitable pairing of elements in spectra, yield the result. ■

To demonstrate the applicability of our general result, we now present its explicit specialization to the case of the Sombor energy.

Corollary 3.15. *Let $G = K_2\square S_n$ for $n \geq 3$, then Sombor energy for graph G is given by:*

$$4(n-2)\sqrt{2}+2\sqrt{4n^3-2n^2+8n-8}.$$

Proof. The result easily follows from Theorem 3.14. Namely, by definition of Sombor matrix $A=\sqrt{n^2+4}$, $B=2\sqrt{2}$ and $C=n\sqrt{2}$, and Sombor energy is given by:

$$\begin{aligned} 4(n-2)\sqrt{2}+&\left|(n+2)\sqrt{2}+\sqrt{4n^3-2n^2+8n-8}\right| \\ &+\left|(n+2)\sqrt{2}-\sqrt{4n^3-2n^2+8n-8}\right|, \end{aligned}$$

and since $n \geq 3$ it reduces to the expression in the corollary formulation. Thus, the proof is completed. ■

Theorem 3.16. *Let $G = K_2\square W_n$ for $n \geq 3$, then*

$$\begin{aligned} &E^{\alpha,\beta,\gamma,\delta}(K_2\square W_n) = BD_{n-1}-4B \\ &+\left|\frac{3B+C+\sqrt{(3B-C)^2+4(n-1)A^2}}{2}\right| + \left|\frac{3B+C-\sqrt{(3B-C)^2+4(n-1)A^2}}{2}\right| \\ &+\left|\frac{B-C+\sqrt{(B+C)^2+4(n-1)A^2}}{2}\right| + \left|\frac{B-C-\sqrt{(B+C)^2+4(n-1)A^2}}{2}\right|, \end{aligned}$$

where $A=\varphi^{\alpha,\beta,\gamma,\delta}(4,n)$, $B=\varphi^{\alpha,\beta,\gamma,\delta}(4,4)$, and $C=\varphi^{\alpha,\beta,\gamma,\delta}(n,n)$, with $\varphi^{\alpha,\beta,\gamma,\delta}$ defined by (3) and D_{n-1} is given in Lemma 3.7.

Proof. The wheel graph W_n can be obtained from the star graph S_n by connecting the leaf vertices to create a cycle of length $n-1$, therefore, we will use graph vertex labeling as described in the proof of Theorem 3.14.

Since the wheel's central vertices in G are of degree n, and all other vertices are of degree 4, using the notation introduced in the formulation of the proposition, the $\Phi-$VDB matrix can be written as:

$$\mathbf{A}^{\alpha,\beta,\gamma,\delta}(K_2\Box W_n) = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{pmatrix},$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & A & A & A & \cdots & A & A \\ A & 0 & B & 0 & \cdots & 0 & B \\ A & B & 0 & B & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & & & \vdots \\ A & B & 0 & 0 & \cdots & B & 0 \end{pmatrix}_{n\times n} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} C & 0 & 0 & \cdots & 0 \\ 0 & B & 0 & \cdots & 0 \\ 0 & 0 & B & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & B \end{pmatrix}_{n\times n}.$$

So, its spectrum can be determined using spectra of $\mathbf{A}+\mathbf{B}$ and $\mathbf{A}-\mathbf{B}$. From (13) we have

$$\begin{aligned} P_{\mathbf{A}+\mathbf{B}}(\lambda) &= det(\mathbf{A}+\mathbf{B}-\lambda\mathbf{I}_n) \\ &= \begin{vmatrix} C-\lambda & A & A & A & \cdots & A & A \\ A & B-\lambda & B & 0 & \cdots & 0 & B \\ A & B & B-\lambda & B & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & & & \vdots \\ A & B & 0 & 0 & \cdots & B & B-\lambda \end{vmatrix} \\ &= A^2 \begin{vmatrix} \frac{C-\lambda}{A^2} & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & B-\lambda & B & 0 & \cdots & 0 & B \\ 1 & B & B-\lambda & B & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & & & \vdots \\ 1 & B & 0 & 0 & \cdots & B & B-\lambda \end{vmatrix} \\ &= A^2\left(\frac{C-\lambda}{A^2} - \mathbf{J}^T\mathbf{R}^{-1}\mathbf{J}\right) det(\mathbf{R}), \end{aligned}$$

where $\mathbf{J}$ is a column vector of length $n-1$ consisting of values 1, and $\mathbf{R}$ is a circulant matrix of order $n-1$ with first row elements $B-\lambda, B, 0, \ldots, 0, B$. Thus, $det(\mathbf{R})$ is the characteristic polynomial of a circulant matrix of order $n-1$ with first row elements $B, B, 0, \ldots, 0, B$, and its spectrum is fully described. It consists of values $B + 2B\cos\frac{2\pi j}{n-1}$, $j = 0, 1, \ldots, n-2$, see, for example, [45] or [46]. Moreover, $\mathbf{J}$ is the eigenvector of the circulant matrix that corresponds to the eigenvalue that is equal to the sum of the raw elements. So, in the case of matrix $\mathbf{R}$, $\mathbf{J}$ is the eigenvector that correspond to the eigenvalue $3B-\lambda$, i.e. $\mathbf{RJ} = (3B-\lambda)\mathbf{J}$, which implies $\mathbf{R}^{-1}\mathbf{J} = \frac{1}{3B-\lambda}\mathbf{J}$. Now, we may write

$$\begin{aligned} P_{\mathbf{A}+\mathbf{B}}(\lambda) &= A^2\left(\frac{C-\lambda}{A^2} - \frac{1}{3B-\lambda}\mathbf{J}^T\mathbf{J}\right) det(\mathbf{R}) \\ &= A^2\left(\frac{C-\lambda}{A^2} - \frac{n-1}{3B-\lambda}\right) det(\mathbf{R}) = \frac{(C-\lambda)(3B-\lambda)-(n-1)A^2}{3B-\lambda} det(\mathbf{R}). \end{aligned}$$

Follows that the spectrum of $\mathbf{A}+\mathbf{B}$ consists of value $B + 2B\cos\frac{2\pi j}{n-1}$, $j = 1, \ldots, n-2$, and values $\left(3B + C \pm \sqrt{(3B-C)^2 + 4(n-1)A^2}\right)/2$, with multiplicity 1.

Analogously,

$$\begin{aligned} P_{\mathbf{A}-\mathbf{B}}(\lambda) &= det(\mathbf{A}-\mathbf{B}-\lambda\mathbf{I}_n) \\ &= A^2\left(\frac{-C-\lambda}{A^2}-\frac{n-1}{B-\lambda}\right)det(\mathbf{Q}) = \frac{(-C-\lambda)(B-\lambda)-(n-1)A^2}{B-\lambda}det(\mathbf{Q}), \end{aligned}$$

where $\mathbf{Q}$ is circulant matrix of order $n-1$ with first row elements $-B-\lambda, B, 0, \dots, 0, B$. So, $det(\mathbf{Q})$ is the characteristic polynomial of circulant matrix of order $n-1$ with first row elements $-B, B, 0, \dots, 0, B$, and its spectrum consists of values $-B+2B\cos\frac{2\pi j}{n-1}$, $j = 0, 1, \dots, n-2$. Conesequently, the spectrum of $\mathbf{A}-\mathbf{B}$ consists of values $-B+2B\cos\frac{2\pi j}{n-1}$, $j = 1, \dots, n-2$ and values $\left(B-C\pm\sqrt{(B+C)^2+4(n-1)A^2}\right)/2$, with multiplicity 1.

All the given facts, combined with Lemma 3.7, yield the result. ■

Explicit specialization of the given result to the case of the Sombor energy is given in the following Corollary.

Corollary 3.17. *Let $G = K_2\Box W_n$ for $n \geq 4$, then Sombor energy for graph G is given by*

$$\sqrt{2}\left(4D_{n-1}-16+\sqrt{2n^3-n^2+8n+112}+\sqrt{2n^3-n^2+40n-16}\right).$$

4 Proof of Lemma 2.2

When $m \geq l$ directly follows that $\left|l\cos\frac{2\pi j}{n}+m\right| = l\cos\frac{2\pi j}{n}+m$ and

$$A_n(l,m) = \sum_{j=0}^{n-1}\left(l\cos\frac{2\pi j}{n}+m\right) = l\sum_{j=0}^{n-1}\cos\frac{2\pi j}{n}+mn.$$

Since

$$\begin{aligned} \sum_{j=0}^{n-1}\cos\frac{2\pi j}{n} &= \sum_{j=0}^{n-1}Re\left(\exp\frac{2\pi ij}{n}\right) \\ &= Re\left(\sum_{j=0}^{n-1}\exp\frac{2\pi ij}{n}\right) = Re\left(\frac{1-\exp(2\pi i)}{1-\exp\frac{2\pi i}{n}}\right) = 0, \end{aligned} \tag{14}$$

we get $A_n(l,m) = mn$ for $m \geq l$. Similarly, $A_n(l,m) = -mn$ when $m \leq -l$.

It is left to evaluate the sum $A_n(l,m)$ when $|m| < l$. Let $J = \{j \in \{0, 1, \dots, n-1\} : l\cos\frac{2\pi j}{n}+m \geq 0\}$. Basic properties of the cosine imply that $J = \{0, 1, \dots, t-1, t\} \cup \{n-t, \dots, n-1\}$, for $t = \lfloor\frac{n}{2\pi}\arccos\left(-\frac{l}{m}\right)\rfloor$. Then,

$$\begin{aligned} A_n(l,m) &= \sum_{j\in J}\left|l\cos\frac{2\pi j}{n}+m\right| + \sum_{j\in\{0,1,\dots,n-1\}\setminus J}\left|l\cos\frac{2\pi j}{n}+m\right| \\ &= \sum_{j\in J}\left(l\cos\frac{2\pi j}{n}+m\right) - \sum_{j\in\{0,1,\dots,n-1\}\setminus J}\left(l\cos\frac{2\pi j}{n}+m\right) \\ &= l\sum_{j\in J}\cos\frac{2\pi j}{n}+m(2t+1) - l\sum_{j\in\{0,1,\dots,n-1\}\setminus J}\cos\frac{2\pi j}{n} - m(n-2t-1), \end{aligned}$$

where in the last step we use the fact that the number of elements in J is equal to $2t+1$ and in its complement to $\{0,1,\ldots,n-1\}$ it is $n-2t-1$. In addition, from (14) follows that

$$\sum_{j\in\{0,1,\ldots,n-1\}\setminus J}\cos\frac{2\pi j}{n}=\sum_{j=0}^{n-1}\cos\frac{2\pi j}{n}-\sum_{j\in J}\cos\frac{2\pi j}{n}=-\sum_{j\in J}\cos\frac{2\pi j}{n},$$

and

$$A_n(l,m) \quad = \quad (4t+2-n)\,m+2l\sum_{j\in J}\cos\frac{2\pi j}{n}. \tag{15}$$

From the definition of the set J and the periodicity of the cosine follows that

$$\sum_{j\in J}\cos\frac{2\pi j}{n}=\sum_{j=-t}^{t}\cos\frac{2\pi j}{n}=1+2\sum_{j=1}^{t}\cos\frac{2\pi j}{n}. \tag{16}$$

Right-hand side expression (16) is the Dirichlet kernel $D_t(x)$, evaluated at $x=\frac{2\pi}{n}$, thus

$$\sum_{j\in J}\cos\frac{2\pi j}{n}=\frac{\sin\left(\left(t+\frac{1}{2}\right)x\right)}{\sin\left(\frac{x}{2}\right)}.$$

This, combined with (15), completes the proof when $|m|<l$. Thus, the lemma is proved.

5 Concluding remarks

This study highlights the inherent complexity of matrix-based molecular descriptors and their associated spectral energies. While refined constructions, such as those underlying the Sombor matrix, aim to enhance discriminative power, analysing energies related to graph products remains challenging due to the strong interdependence encoded in the corresponding matrices. The unified formulation considered here allows the systematic investigation of the underlying matrices and their spectra while enabling continuous parameter variation, which may reveal the influence of individual terms. Furthermore, the framework employed is not restricted to degree-based constructions and can naturally be extended to matrices defined via other vertex characteristics, thereby enhancing its applicability.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

Appendix A: Topological indices

Name	The corresponding symmetric function	Parameters $(\alpha, \beta, \gamma, \delta)$ from (3)	Index defined in	Energy-related studies
AG (arithmetic-geometric)	$(d_i + d_j)/(2\sqrt{d_i d_j})$	$\left(-1, \frac{1}{2}, \frac{1}{2}, 0\right)$	[47]	[48, 49]
Euler-Sombor	$\sqrt{d_i^2 + d_j^2 + d_i d_j}$	$\left(2, \frac{1}{2}, 0, 1\right)$	[30]	[30]
Forgotten	$d_i^2 + d_j^2$	$(2, 1, 0, 0)$	[50, 51]	[52]
GA (geometric-arithmetic)	$2\sqrt{d_i d_j}/(d_i + d_j)$	$\left(-1, -\frac{1}{2}, -\frac{1}{2}, 0\right)$	[53]	[54–56]
Gourava (first)	$(d_i + d_j + d_i d_j)$	$(1, 1, 0, 1)$	[57]	[58]
Gourava (second)	$(d_i + d_j) d_i d_j$	$(-1, -1, 2, 0)$	[57]	[58]
Harmonic	$2/(d_i + d_j)$	$(0, 1, -1, 0)$	[59]	[52, 55, 56]
Inverse degree	$d_i^{-2} + d_j^{-2}$	$(-2, 1, 0, 0)$	[59, 60]	
Inverse sum	$d_i d_j/(d_i + d_j)$	$(-1, -1, 0, 0)$	[61]	[56, 62]
Nirmala	$\sqrt{d_i + d_j}$	$\left(1, 0, \frac{1}{2}, 0\right)$	[63]	[56, 64]
Randić	$1/\sqrt{d_i d_j}$	$\left(-1, \frac{1}{2}, -\frac{1}{2}, 0\right)$	[65]	[66–71]
Randić (second)	$1/(d_i d_j)$	$(-1, 1, -1, 0)$	[65, 72]	[56, 73]
Randić, generalized	$(d_i d_j)^{\mathtt{p}},\ \mathtt{p} \in \mathbb{R}$	$(-1, -\mathtt{p}, \mathtt{p}, 0)$	[72]	[56, 73]
Randić, reciprocal	$\sqrt{d_i d_j}$	$\left(-1, -\frac{1}{2}, \frac{1}{2}, 0\right)$	[72, 74]	[56, 73]
Sombor	$\sqrt{(d_i^2 + d_j^2)}$	$\left(2, \frac{1}{2}, 0, 0\right)$	[7]	[26]
Sombor, diminished	$\frac{\sqrt{d_i^2 + d_j^2}}{d_i + d_j}$	$\left(2, \frac{1}{2}, -1, 0\right)$	[32]	[32]
Sombor, elliptic	$(d_i + d_j)\sqrt{d_i^2 + d_j^2}$	$\left(2, \frac{1}{2}, 1, 0\right)$	[29]	[29]
Sombor, modified	$\frac{1}{\sqrt{d_i^2 + d_j^2}}$	$\left(2, -\frac{1}{2}, 0, 0\right)$	[3]	[3]
$\mathtt{p}$-Sombor	$(d_i^{\mathtt{p}} + d_j^{\mathtt{p}})^{1/\mathtt{p}}$	$\left(\mathtt{p}, \frac{1}{\mathtt{p}}, 0, 0\right)$	[31]	[31]
Sum-connectivity	$1/\sqrt{d_i + d_j}$	$\left(1, 0, -\frac{1}{2}, 0\right)$	[75]	[56]
Zagreb (first)	$d_i + d_j$	$(1, 0, 1, 0)$	[51]	[76, 77]
Zagreb (second)	$d_i d_j$	$(-1, -1, 1, 0)$	[78]	[76]
hyper-Zagreb (first)	$(d_i + d_j)^2$	$(1, 0, 2, 0)$	[79]	

Table 2: Topological indices, the corresponding function, the values of parameters, and some related references.

To obtain equality, the function with the given parameters has to be multiplied by 1/2.
To obtain equality, the function with the given parameters has to be multiplied by 2.

Appendix B: $\Phi-$VDB energies for selected graphs

Name	Cyclic graph C_n	Complete graph K_n	Star graph S_n	Complete bipartite graph $K_{p,q}$
AG (arithmetic–geometric)	$2A_n$	$2(n-1)$	n	$p+q$
Euler–Sombor	$4\sqrt{3}A_n$	$2\sqrt{3}(n-1)^2$	$2\sqrt{(n-1)((n-1)^2+n)}$	$2\sqrt{pq(p^2+pq+q^2)}$
Forgotten	$16A_n$	$4(n-1)^3$	$2((n-1)^2+1)\sqrt{n-1}$	$2\sqrt{pq}(p^2+q^2)$
GA (geometric–arithmetic)	$2A_n$	$2(n-1)$	$4-\frac{4}{n}$	$\frac{4pq}{p+q}$
Gourava (first)	$16A_n$	$2(n-1)(n^2-1)$	$2\sqrt{n-1}(2n-1)$	$2\sqrt{pq}(pq+p+q)$
Gourava (second)	$32A_n$	$4(n-1)^4$	$2(n-1)^{3/2}n$	$2(pq)^{3/2}(p+q)$
Harmonic	A_n	2	$\frac{4\sqrt{n-1}}{n}$	$\frac{4\sqrt{pq}}{p+q}$
Inverse degree	A_n	$\frac{4}{n-1}$	$2\left(1+\frac{1}{(n-1)^2}\right)\sqrt{n-1}$	$\frac{2(p^2+q^2)}{(pq)^{3/2}}$
Inverse sum	$2A_n$	$(n-1)^2$	$\frac{2(n-1)^{3/2}}{n}$	$\frac{2(pq)^{3/2}}{p+q}$
Nirmala	$4A_n$	$2\sqrt{2}(n-1)^{3/2}$	$2\sqrt{(n-1)n}$	$2\sqrt{pq(p+q)}$
Randić	A_n	2	2	2
Randić (second)	$\frac{A_n}{2}$	$\frac{2}{n-1}$	$\frac{2}{\sqrt{n-1}}$	$\frac{2}{\sqrt{pq}}$
Randić, generalized	$2^{2p+1}A_n$	$2(n-1)^{2p+1}$	$2(n-1)^{p+\frac{1}{2}}$	$2(pq)^{p+\frac{1}{2}}$
Randić, reciprocal	$4A_n$	$2(n-1)^2$	$2(n-1)$	$2pq$
Sombor	$4\sqrt{2}A_n$	$2\sqrt{2}(n-1)^2$	$2\sqrt{((n-1)^2+1)(n-1)}$	$2\sqrt{pq(p^2+q^2)}$
Sombor, diminished	$\sqrt{2}A_n$	$\sqrt{2}(n-1)$	$\frac{2\sqrt{(n-1)((n-2)n+2)}}{n}$	$\frac{2\sqrt{pq(p^2+q^2)}}{p+q}$
Sombor, elliptic	$16\sqrt{2}A_n$	$4\sqrt{2}(n-1)^3$	$2n\sqrt{((n-1)^2+1)(n-1)}$	$2(p+q)\sqrt{pq(p^2+q^2)}$
Sombor, modified	$\frac{A_n}{\sqrt{2}}$	$\sqrt{2}$	$2\sqrt{\frac{n-1}{(n-2)n+2}}$	$2\sqrt{\frac{pq}{p^2+q^2}}$
$\mathtt{p}$-Sombor	$2^{2+\frac{1}{\mathtt{p}}}A_n$	$2^{1+\frac{1}{\mathtt{p}}}(n-1)^2$	$2((n-1)^{\mathtt{p}}+1)^{1/\mathtt{p}}\sqrt{n-1}$	$2\sqrt{pq}\,(p^{\mathtt{p}}+q^{\mathtt{p}})^{1/\mathtt{p}}$
Sum-connectivity	A_n	$\sqrt{2}\sqrt{n-1}$	$2\sqrt{\frac{n-1}{n}}$	$2\sqrt{\frac{pq}{p+q}}$
Zagreb (first)	$8A_n$	$4(n-1)^2$	$2\sqrt{n-1}\,n$	$2\sqrt{pq}(p+q)$
Zagreb (second)	$8A_n$	$2(n-1)^3$	$2(n-1)^{3/2}$	$2(pq)^{3/2}$
hyper-Zagreb (first)	$32A_n$	$8(n-1)^3$	$2\sqrt{n-1}n^2$	$2\sqrt{pq}(p+q)^2$

Table 3: $\Phi-$VDB energies of cyclic, complete, star and complete bipartite graphs.

Appendix C: $\Phi-$VDB energies for selected graph products

Name	$K_p \Box K_q$	$K_p \otimes K_q$
AG (arithmetic–geometric)	$4(p-1)(q-1)$	$4(p-1)(q-1)$
Euler–Sombor	$4\sqrt{3}(p-1)(q-1)(p+q-2)$	$4\sqrt{3}(p-1)^2(q-1)^2$
Forgotten	$8(p-1)(q-1)(p+q-2)^2$	$8(p-1)^3(q-1)^3$
GA (geometric–arithmetic)	$4(p-1)(q-1)$	$4(p-1)(q-1)$
Gourava (first)	$4(p-1)(q-1)(p+q-2)(p+q)$	$4(p-1)^2(p(q-1)-q+3)(q-1)^2$
Gourava (second)	$8(p-1)(q-1)(p+q-2)^3$	$8(p-1)^4(q-1)^4$
Harmonic	$\frac{4(p-1)(q-1)}{p+q-2}$	4
Inverse degree	$\frac{8(p-1)(q-1)}{(p+q-2)^2}$	$\frac{8}{(p-1)(q-1)}$
Inverse sum	$2(p-1)(q-1)(p+q-2)$	$2(p-1)^2(q-1)^2$
Nirmala	$4\sqrt{2}(p-1)(q-1)\sqrt{p+q-2}$	$4\sqrt{2}((p-1)(q-1))^{3/2}$
Randić	$\frac{4(p-1)(q-1)}{p+q-2}$	4
Randić (second)	$\frac{4(p-1)(q-1)}{(p+q-2)^2}$	$\frac{4}{(p-1)(q-1)}$
Randić, generalized	$4(p-1)(q-1)(p+q-2)^{2p}$	$4((p-1)(q-1))^{2p+1}$
Randić, reciprocal	$4(p-1)(q-1)(p+q-2)$	$4(p-1)^2(q-1)^2$
Sombor	$4\sqrt{2}(p-1)(q-1)(p+q-2)$	$4\sqrt{2}(p-1)^2(q-1)^2$
Sombor, diminished	$2\sqrt{2}(p-1)(q-1)$	$2\sqrt{2}(p-1)(q-1)$
Sombor, elliptic	$8\sqrt{2}(p-1)(q-1)(p+q-2)^2$	$8\sqrt{2}(p-1)^3(q-1)^3$
Sombor, modified	$\frac{2\sqrt{2}(p-1)(q-1)}{p+q-2}$	$2\sqrt{2}$
p-Sombor	$2^{2+\frac{1}{\mathrm{p}}}(p-1)(q-1)(p+q-2)$	$2^{2+\frac{1}{\mathrm{p}}}(p-1)^2(q-1)^2$
Sum-connectivity	$\frac{2\sqrt{2}(p-1)(q-1)}{\sqrt{p+q-2}}$	$2\sqrt{2}\sqrt{(p-1)(q-1)}$
Zagreb (first)	$8(p-1)(q-1)(p+q-2)$	$8(p-1)^2(q-1)^2$
Zagreb (second)	$4(p-1)(q-1)(p+q-2)^2$	$4(p-1)^3(q-1)^3$
hyper-Zagreb (first)	$16(p-1)(q-1)(p+q-2)^2$	$16(p-1)^3(q-1)^3$

Table 4: $\Phi-$VDB energies of Cartesian product $K_p \Box K_q$ and direct product $K_p \otimes K_q$.

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