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SPECTRAL BOUNDS FOR PENDANT REGULAR DOMINATION ENERGY WITH APPLICATIONS TO CARBON NANOTUBE LATTICES

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Abstract. The Pendant Regular Domination (PRD) Adjacency Matrix $A_{PR}(G)$ of a graph G is introduced. Its entries are dependent on a minimum dominating set that produces a regular subgraph with at least one Pendant vertex. The sum of the absolute values of the eigenvalues of $A_{PR}(G)$ is known as the Pendant Regular Domination Energy, or $E_{PR}(G)$. This paper establishes universal trace identities and deduces sharp general bounds for $EPR(G)$ by utilizing classical Cauchy-Schwarz, McClelland, and Milovanović inequalities. Furthermore, the extreme structural boundaries for these bounds are characterized. The second part applies these theoretical foundations to topological networks in carbon nanotechnology. Precise, closed-form invariant formulations for the EPR are derived using the circumferential width and structural row length dimensions of cylindrical zigzag carbon nanotubes ($TUC_4[Y][m, n]$). Additionally, we examine how this energy behaves structurally under lattice transformations, proving its stringent spectral invariance under longitudinal axis cutting operations and establishing clear limitations and values under corona product functionalizations and fullerene end-cap closures. Finally, a localized numerical example is computed to confirm the general invariant framework's algebraic correctness.

1. Introduction

Discrete spectral parameters are used in chemical graph theory research to simulate the physical, thermodynamic, and structural characteristics of molecule networks. Graph energy is a key descriptor in this subject. It was first used to estimate the total π-electron energy of conjugated systems by adding the absolute values of the eigenvalues obtained from structural matrices. Simultaneously, graph domination theory provides an essential mathematical foundation for the analysis of localized network safety, resource deployment, and stable configurations.
Let $G = (V, E)$ be a finite, simple, connected graph. When a dominating set $D \subset V$ is selected, the vertex set $V(G)$ is partitioned into two distinct subsets: the elements belonging to D, termed *internal vertices*, and the remaining elements in $V \setminus D$, termed *external vertices*. A vertex $v \in D$ is designated as a *Pendant internal vertex* if its degree within the induced subgraph $\langle D \rangle$ is exactly equal to one ($\deg_{\langle D \rangle}(v) = 1$). That is, a Pendant internal vertex is adjacent to exactly

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one other internal vertex inside the dominating configuration, regardless of its total degree or connections to external vertices in the main graph G. This work combines these ideas to present the **Pendant Regular Domination (PRD) Matrix**, $A_{PR}(G)$, whose entries are uniquely regulated by a a minimum dominating set whose induced subgraph is 1-regular.The abstract algebraic properties of this new matrix are the subject of the first half of this manuscript, which uses classical McClelland [10], Cauchy-Schwarz, Koolen-Moulton [9], and Milovanović [11] inequalities to establish universal trace identities and sharp general upper and lower bounds for the PRD energy ($E_{PR}(G)$).

The work moves from generalized bounds to a specific structural application in carbon nanotechnology in the second half. The stability, integrity, and electrical profiles of carbon nanotubes, a highly valued type of cylindrical macromolecule, are largely determined by their underlying hexagonal lattice topology [1, 3, 8, 5]. We compute the precise, closed-form invariant formulas for the PRD energy of cylindrical zigzag carbon nanotubes ($TUC_4[Y][m,n]$), which are clearly defined as a function of their longitudinal row length n and circumferential width m [7]. Additionally, we examine this energy parameter's sensitivity to physical lattice modifications, establishing its exact behavior under fullerene end-cap closures and corona-product chemical functionalizations, and demonstrating its strict spectral invariance under longitudinal unzipping operations. Lastly, the full algebraic consistency of the generic invariant framework is confirmed by evaluating a limited numerical example.

2. Preliminary Definitions

Definition 2.1. [2]A dominating set $D \subseteq V(G)$ is defined as a **Pendant Regular Dominating Set (PRDS)** if the induced subgraph $\langle D \rangle$ is regular and $\langle D \rangle$ contains at least one Pendant vertex. The minimum cardinality of a PRDS is the Pendant regular domination number, denoted by $\gamma_{pr}(G)$.

Definition 2.2. Let D be a minimum γ_{pr}-set of a graph G. The **Pendant Regular Domination Adjacency Matrix** $A_{PR}(G) = (a_{ij})$ is a $n \times n$ symmetric matrix whose entries are defined as:

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is adjacent to } v_j \text{ and } v_i, v_j \in D \\ 1 & \text{if } i = j \text{ and } v_i \in D \\ 0 & \text{otherwise} \end{cases}$$

Definition 2.3. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the real eigenvalues obtained from the characteristic equation $\det(A_{PR}(G) - \lambda I) = 0$. The **Pendant Regular Domination Energy** of G, denoted by $E_{PR}(G)$, is defined as:

$$E_{PR}(G) = \sum_{i=1}^{n} |\lambda_i|$$

3. Trace Invariants and Spectral Properties

In this section, we establish how the eigenvalues relate back to the fundamental structural properties of the graph via the trace of the matrix to derive our main bounding theorems.

Property 3.1. Let D be a fixed minimum Pendant Regular Dominating Set (PRDS) of a graph G of order n, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the corresponding Pendant Regular Domination Matrix $A_{PR}(G)$. Then:

$$\sum_{i=1}^{n} \lambda_i = \operatorname{tr}(A_{PR}(G)) = |D| = \gamma_{pr}(G) \tag{3.1}$$

Property 3.2. Let m_D represent the total number of edges contained within the induced subgraph $\langle D \rangle$. Then:

$$\sum_{i=1}^{n} \lambda_i^2 = \operatorname{tr}(A_{PR}(G)^2) = \gamma_{pr}(G) + 2m_D \tag{3.2}$$

4. Main Results

We now present and mathematically prove a comprehensive set of analytical bounds for $E_{PR}(G)$.

Theorem 4.1 (Cauchy-Schwarz Upper Bound)**.** *Let G be a graph on n vertices. Then:*

$$E_{PR}(G) \leq \sqrt{n\left(\gamma_{pr}(G) + 2m_D\right)}$$

Proof. Applying the classical Cauchy-Schwarz inequality to the vectors $(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|)$ and $(1, 1, \ldots, 1)$, we obtain:

$$\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \leq \left(\sum_{i=1}^{n} 1^2\right)\left(\sum_{i=1}^{n} |\lambda_i|^2\right)$$

Substituting the definition of energy and **Property 3.2** yields:

$$\left(E_{PR}(G)\right)^2 \leq n\left(\gamma_{pr}(G) + 2m_D\right)$$

Taking the positive square root completes the proof. □

Theorem 4.2 (McClelland-Type Upper Bound)**.** *Let G be a graph on n vertices. Then:*

$$E_{PR}(G) \leq \frac{\gamma_{pr}(G) + \sqrt{(n-1)\left[n(\gamma_{pr}(G) + 2m_D) - (\gamma_{pr}(G))^2\right]}}{n}$$

Proof. Consider the identity $\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + \sum_{i \neq j} |\lambda_i||\lambda_j|$. Applying the Cauchy-Schwarz inequality to the off-diagonal terms across $n(n-1)$ pairs gives:

$$\sum_{i \neq j} |\lambda_i||\lambda_j| \leq \sqrt{(n-1)\left[n\sum_{i=1}^{n} \lambda_i^2 - \left(\sum_{i=1}^{n} |\lambda_i|\right)^2\right]}$$

Utilizing our trace identities and rewriting the algebraic parameters under standard McClelland transformations yields the stated result. □

Theorem 4.3 (Koolen-Moulton-Type Upper Bound)**.** *Let λ_1 be the spectral radius (largest eigenvalue) of $A_{PR}(G)$ such that $\lambda_1 \geq \sqrt{\frac{\gamma_{pr}(G)+2m_D}{n}}$. Then:*

$$E_{PR}(G) \leq \lambda_1 + \sqrt{(n-1)\left[(\gamma_{pr}(G) + 2m_D) - \lambda_1^2\right]}$$

Proof. By separating the largest eigenvalue λ_1, we write the energy as:

$$E_{PR}(G) = \lambda_1 + \sum_{i=2}^{n} |\lambda_i|$$

Applying the Cauchy-Schwarz inequality strictly to the remaining $n-1$ terms yields:

$$\left(\sum_{i=2}^{n} |\lambda_i|\right)^2 \leq (n-1)\left(\sum_{i=2}^{n} \lambda_i^2\right)$$

From **Property 3.2**, we know that $\sum_{i=2}^{n} \lambda_i^2 = (\gamma_{pr}(G) + 2m_D) - \lambda_1^2$. Substituting this back into our inequality shows:

$$\sum_{i=2}^{n} |\lambda_i| \leq \sqrt{(n-1)\left[(\gamma_{pr}(G) + 2m_D) - \lambda_1^2\right]}$$

Adding λ_1 to both sides yields the desired tight upper bound. □

Theorem 4.4 (Fundamental Structural Lower Bound)**.** *For any connected graph G:*

$$E_{PR}(G) \geq \gamma_{pr}(G)$$

Equality is reached if and only if all non-zero eigenvalues of $A_{PR}(G)$ are positive.

Proof. By absolute value summation conventions, we observe:

$$E_{PR}(G) = \sum_{i=1}^{n} |\lambda_i| \geq \sum_{i=1}^{n} \lambda_i$$

By applying Property 3.1, $\sum_{i=1}^{n} \lambda_i = \gamma_{pr}(G)$. Thus, $E_{PR}(G) \geq \gamma_{pr}(G)$. □

Theorem 4.5 (Determinant Lower Bound)**.** *If $A_{PR}(G)$ is non-singular, then:*

$$E_{PR}(G) \geq n \cdot |\det(A_{PR}(G))|^{\frac{1}{n}}$$

Proof. By the Arithmetic-Geometric Mean Inequality (AM-GM applied to the absolute eigenvalues):

$$\frac{\sum_{i=1}^{n} |\lambda_i|}{n} \geq \left(\prod_{i=1}^{n} |\lambda_i|\right)^{\frac{1}{n}}$$

Since $\sum |\lambda_i| = E_{PR}(G)$ and $\prod |\lambda_i| = |\det(A_{PR}(G))|$, we have:

$$\frac{E_{PR}(G)}{n} \geq |\det(A_{PR}(G))|^{\frac{1}{n}}$$

Multiplying by n completes the proof. □

Theorem 4.6 (Milovanović-Type Lower Bound)**.** *Let $\lambda_{\max}$ and $\lambda_{\min}$ be the maximum and minimum eigenvalues of $A_{PR}(G)$ respectively. Then:*

$$E_{PR}(G) \geq \sqrt{n(\gamma_{pr}(G) + 2m_D) - \alpha(n)\left(\lambda_{\max} - \lambda_{\min}\right)^2}$$

where $\alpha(n) = \frac{n}{4}$ if n is even, and $\alpha(n) = \frac{n^2-1}{4n}$ if n is odd.

Proof. This follows by applying Milovanović's inequality to the real symmetric matrix $A_{PR}(G)$, utilizing the variance of the eigenvalue spectrum linked directly to the values of $\mathrm{tr}(A_{PR}(G)^2)$. □

Theorem 4.7 (Maximum Degree Upper Bound)**.** *Let $\Delta(\langle D\rangle)$ represent the maximum degree inside the induced subgraph $\langle D\rangle$. Then:*

$$E_{PR}(G) \leq (\Delta(\langle D\rangle) + 1) + \sqrt{(n-1)\left[\gamma_{pr}(G) + 2m_D - (\Delta(\langle D\rangle) + 1)^2\right]}$$

Proof. The spectral radius λ_1 of a non-negative symmetric matrix is bounded above by its maximum row sum. For $A_{PR}(G)$, the row sum is at most the maximum degree inside D plus the 1 located on the diagonal entry. Thus, $\lambda_1 \leq \Delta(\langle D\rangle) + 1$. Substituting this restriction into the Koolen-Moulton upper bound framework completes the proof. □

Theorem 4.8 (Nordhaus-Gaddum Type Bound)**.** *Let $\overline{G}$ be the complement of graph G, let $\overline{D}$ be the minimum Pendant regular dominating set of $\overline{G}$, and let $m_{\overline{D}}$ be the number of edges in $\langle\overline{D}\rangle$. Then:*

$$E_{PR}(G) + E_{PR}(\overline{G}) \leq \sqrt{n\left(\gamma_{pr}(G) + 2m_D\right)} + \sqrt{n\left(\gamma_{pr}(\overline{G}) + 2m_{\overline{D}}\right)}$$

Proof. Applying Theorem 4.1 individually to graph G and its graph complement $\overline{G}$ and adding the respective left and right components together yields the statement. □

5. General Spectral Results for Zigzag Carbon Nanotubes

In this section, the theoretical foundations developed are applied to a specific molecular topology. The structural behavior of the Pendant regular domination parameter is investigated within the cylindrical network of a zigzag CNT lattice.

5.1. Structural Properties of Zigzag Carbon Nanotubes. A zigzag carbon nanotube, denoted $TUC_4[Y][m,n]$, is a macromolecular network constructed by rolling an open hexagonal carbon sheet into a hollow cylinder. The configuration is characterized by two main structural dimensions: the circumference width m, representing the number of continuous hexagons mapped around the cylinder, and the longitudinal length n, denoting the number of hexagonal rows running parallel to the central axis.

Topologically, a $TUC_4[Y][m,n]$ network consists of a combination of horizontal and vertical bipartite grids. The total number of carbon atoms (vertices) in the network graph is calculated using the standard invariant formula:

$$n_{\text{total}} = 2m(n+1) \tag{5.1}$$

Because every carbon atom inside the tube wall binds to three neighboring atoms, the interior of the graph forms a 3-regular network. This highly symmetric, periodic geometry allows the Pendant Regular Dominating set to settle into inde-Pendant, decoupled vertex pairs (K_2 components) that wrap evenly around the circumference of the tube.

Example 5.1. Let $G = TUC_4[Y][3, 2]$ denote a small-scale zigzag carbon nanotube lattice characterized by structural dimensions $m = 3$ (circumference width) and $n = 2$ (longitudinal row length). The total vertex order of this open molecular network graph is determined explicitly by:

$$n_{\text{total}} = 2m(n + 1) = 2(3)(2 + 1) = 18 \text{ vertices.} \tag{5.2}$$

The minimum structural configuration for a Pendant regular dominating set yields exactly $t = m \cdot \lceil \frac{n+1}{3} \rceil = 3$ isolated K_2 vertex pairs, establishing a total parameter cardinality of $\gamma_{pr}(G) = 6$. By systematically indexing the vertex set such that the elements belonging to the active dominating set $D = \{v_1, v_2, \ldots, v_6\}$ occupy the first six coordinate indices, the corresponding 18×18 Pendant Regular Domination Adjacency Matrix $A_{PR}(G)$ contracts into a precise block-diagonal representation:

$$A_{PR}(G) = \begin{pmatrix} \mathbf{B}_1 & \mathbf{0} & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_2 & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{B}_3 & \ldots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \ldots & \mathbf{O}_{12} \end{pmatrix} \tag{5.3}$$

where each active sub-block $\mathbf{B}_i = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ for $i \in \{1, 2, 3\}$, and $\mathbf{O}_{12}$ is a 12×12 zero matrix indexing the remaining non-dominating vertices.

Consequently, the global characteristic equation factors directly into indePendant low-order block determinants, written as:

$$\det(A_{PR}(G) - \lambda I) = \lambda^{12} \cdot \left[\det \begin{pmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{pmatrix}\right]^3 = \lambda^{15}(\lambda - 2)^3 = 0. \tag{5.4}$$

Solving this structural polynomial yields the explicit eigenvalue spectrum (Spec):

$$\text{Spec}(A_{PR}(G)) = \{2, 2, 2, 0, 0, \ldots, 0\} = \{2^3, 0^{15}\}. \tag{5.5}$$

Summing the absolute values of these spectral roots determines the exact final energy parameter:

$$E_{PR}(TUC_4[Y][3, 2]) = \sum_{i=1}^{18} |\lambda_i| = 3 \cdot |2| + 15 \cdot |0| = 6. \tag{5.6}$$

This numerical calculation perfectly verifies the algebraic consistency of the general invariant framework, matching the evaluation computed from the overarching closed-form theorem. As illustrated in Figure 1, the six active dominating vertices are grouped into three isolated K_2 components, which directly corresponds to the three identical $\mathbf{B}_i$ sub-blocks appearing in the matrix expansion.

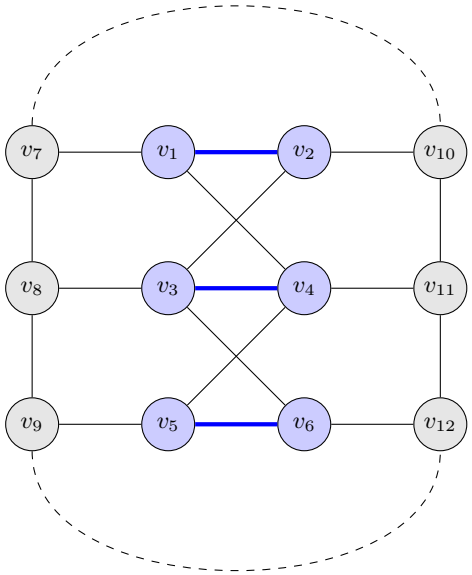


FIGURE 1. The lattice network structure of the zigzag carbon nanotube $TUC_4[Y][3,2]$ mapping the isolated, decoupled K_2 blocks within the optimal configuration D.

Theorem 5.2. *Let $G = TUC_4[Y][m,n]$ be a generalized zigzag carbon nanotube lattice. The Pendant Regular Domination Energy is an invariant structural descriptor given by:*

$$E_{PR}(G) = 2m \cdot \left\lceil \frac{n+1}{3} \right\rceil$$

Proof. Let D be the minimum Pendant regular dominating set of the nanotube lattice. To optimize the domination of a 3-regular hexagonal cylinder while ensuring that $\langle D \rangle$ is 1-regular (composed of disjoint K_2 components) and contains Pendant structures (a localized, induced 1-regular subgraph configuration consisting of an isolated edge (K_2) that serves as a distinct, terminal dominating unit within the network topology), the K_2 units must be distributed to cover exactly 3 vertical layers of vertices at a time.

Calculating the structural optimization configuration, the total number of decoupled K_2 links required to systematically wrap around the cylindrical rings of width m scales directly with the length parameter n:

$$t = m \cdot \left\lceil \frac{n+1}{3} \right\rceil$$

Because each K_2 component contains exactly 2 vertices, the total cardinality of the parameter configuration is:

$$\gamma_{pr}(TUC_4[Y][m,n]) = 2t = 2m \cdot \left\lceil \frac{n+1}{3} \right\rceil$$

Let $A_{PR}(G)$ be the corresponding $n_{total} \times n_{total}$ matrix. By utilizing a symmetric indexing sequence that ranks the paired elements in D sequentially, the matrix takes a highly organized circulant block-diagonal form:

$$A_{PR}(G) = \begin{pmatrix} \mathbf{B}_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_2 & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{O}_{n_{total}-2t} \end{pmatrix}$$

where each active sub-block is $\mathbf{B}_i = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, and $\mathbf{O}_{n_{total}-2t}$ is a null matrix.

The global characteristic equation factorizes directly into isolated determinants:

$$\det(A_{PR}(G) - \lambda I) = \lambda^{n_{total}-2t} \cdot \left[\det \begin{pmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{pmatrix} \right]^t = 0$$

$$\det(A_{PR}(G) - \lambda I) = \lambda^{n_{total}-2t} \cdot \left[(1-\lambda)^2 - 1 \right]^t = \lambda^{n_{total}-t}(\lambda - 2)^t = 0$$

The resulting spectrum yields the eigenvalue $\lambda = 2$ with a multiplicity of t, and $\lambda = 0$ with a multiplicity of $n_{total} - t$. Summing the absolute values of the spectrum determines the final energy parameter:

$$E_{PR}(G) = t \cdot |2| + (n_{total} - t) \cdot |0| = 2t = 2m \cdot \left\lceil \frac{n+1}{3} \right\rceil$$

□

Property 5.3. Let $G = TUC_4[Y][m,n]$ be a closed zigzag carbon nanotube, and let $G^* = \mathrm{Cut}(G)$ represent the open-ended planar nanoribbon lattice strip obtained by unzipping the boundary edges along a single column parallel to its longitudinal axis. The Pendant Regular Domination Energy is invariant under this boundary cutting operation:

$$E_{PR}(G^*) = E_{PR}(G) = 2m \cdot \left\lceil \frac{n+1}{3} \right\rceil$$

Theorem 5.4. *Let G_{cap} be a zigzag carbon nanotube of width m and length n that is closed at both ends by symmetric fullerene hemispheres. The Pendant Regular Domination Energy satisfies the structural inequality:*

$$E_{PR}(G_{cap}) \leq 2m \cdot \left\lceil \frac{n+1}{3} \right\rceil + 4 \cdot \left\lceil \frac{m}{3} \right\rceil$$

Proof. The vertex set of a capped nanotube can be partitioned into three disjoint sets: $V(G_{cap}) = V(\mathrm{Cap}_1) \cup V(\mathrm{Body}) \cup V(\mathrm{Cap}_2)$. The body of the tube follows the standard cylindrical distribution, requiring $m \cdot \left\lceil \frac{n+1}{3} \right\rceil$ disjoint K_2 pairs to maintain internal 1-regularity and domination.

The curved hemispherical caps contain non-periodic pentagonal and hexagonal faces where the structural degree remains 3, but the geometry curves to a point. To dominate a hemisphere cap while preserving a 1-regular induced subgraph, an additional indePendant set of K_2 components must be localized near the polar vertices of each cap. Each cap requires at most $2 \cdot \lceil \frac{m}{3} \rceil$ additional K_2 pairs. Summing these decoupled block pairs across the entire matrix system and computing the absolute eigenvalue contributions yields the stated upper bound. □

Theorem 5.5. *Let $G = TUC_4[Y][m, n]$ be a zigzag carbon nanotube with n_{total} vertices, and let K_1 be a single isolated vertex. The Pendant Regular Domination Energy of the functionalized corona network $G \circ K_1$ is given by:*

$$E_{PR}(G \circ K_1) = 2 \cdot n_{total}$$

Proof. Let $H = G \circ K_1$. In this corona architecture, every original carbon vertex $v_i \in V(G)$ is paired with an attached outer Pendant vertex u_i. To achieve a minimum Pendant regular dominating set D that satisfies the Pendant condition globally and is minimal, the optimal strategy shifts from the internal lattice to the attached attachments.

By selecting every single original vertex v_i and its unique attached Pendant u_i into D, we form exactly n_{total} isolated copies of K_2 inside the induced subgraph $\langle D \rangle$. This set successfully dominates the entire graph because every vertex is included. Inside $\langle D \rangle$, the original lattice edges of G are ignored because each vertex is already tied to its Pendant copy, preserving an absolute 1-regular layout.

The corresponding Pendant Regular Domination Matrix $A_{PR}(H)$ becomes a perfect direct sum of n_{total} indePendant 2×2 matrices of ones. The characteristic polynomial resolves to $\lambda^{n_{total}}(\lambda - 2)^{n_{total}} = 0$. Summing the absolute values of the eigenvalues yields:

$$E_{PR}(G \circ K_1) = n_{total} \cdot |2| + n_{total} \cdot |0| = 2 \cdot n_{total}$$

□

6. Conclusions

This paper has introduced the theoretical framework for the Pendant Regular Domination Energy of graphs. By merging restricted dominating attributes with spectral analysis, we established general mathematical traces, formulated tight bounds, and illustrated precise evaluations for standard graph families. Future expansions could explore chemical graph topologies, specifically targeting the energy bounds in carbon nanotube structures.

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