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A Computational Analysis of Spectral Properties and Energies of Distance-Based Matrices for Selected Hydrocarbons

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Abstract

This paper extends the spectral analysis of distance-based matrices associated with chemical graph structures of order n, focusing on the distance matrix $\mathcal{D}(\mathcal{G})$, the distance Laplacian $\mathcal{DL}(\mathcal{G})$, and the distance signless Laplacian $\mathcal{DQ}(\mathcal{G})$. We investigate the spectral integrality of these matrices for selected acyclic and cyclic hydrocarbon molecular graphs by examining whether their corresponding spectra consist entirely of integers. In addition, we compute and compare the associated distance energies, namely, the distance energy $\mathcal{E}_{\mathcal{D}}$, the distance Laplacian energy $\mathcal{E}_{\mathcal{DL}}$, and the distance signless Laplacian energy $\mathcal{E}_{\mathcal{DQ}}$ to explore their structural significance. Using computational tools, we present numerical results and graphical comparisons that reveal meaningful relationships among these energies. In particular, our analysis establishes the conjecture in the form of a strict inequality $\mathcal{E}_{\mathcal{DL}} > \mathcal{E}_{\mathcal{DQ}} > \mathcal{E}_{\mathcal{D}}$. These findings demonstrate that the distance Laplacian energy is more sensitive to molecular structural variations, highlighting its effectiveness as a discriminative molecular descriptor in chemical graph theory.

Keywords: chemical graph theory; distance matrix; distance Laplacian; distance signless Laplacian; integral spectrum; linear algebra

1. Introduction

Graphs are powerful tools in linear algebra and chemistry, representing molecular structures where vertices correspond to atoms and edges to chemical bonds. Chemical graph theory models molecular structures as graphs, enabling the study of chemical properties through spectral methods.

The following definitions are adapted from [1] and standard graph theory literature, with emphasis on linear algebra and chemical graph applications. Let $\mathcal{G} = (V(\mathcal{G}), E(\mathcal{G}))$ be a connected, undirected, simple graph with vertex set $V(\mathcal{G}) = v_1, \ldots, v_n$ and edge set $E(\mathcal{G})$, where vertices and edges represent atoms and chemical bonds, respectively. For $v_i, v_j \in V(\mathcal{G})$, $d_{ij} = d_{\mathcal{G}}(v_i, v_j)$ denotes the length of the shortest path between them. The *transmission* of a vertex v_i, denoted $\mathcal{T}(\mathcal{G})_{i,i}$, is defined as the sum of distances from v_i to all other vertices:

$$\mathcal{T}(\mathcal{G})_{i,i} = \sum_{j=1}^{n} d_{ij}. \tag{1}$$

where d_{ij} is the (i, j)-th element of $\mathcal{D}(\mathcal{G})$. The transmission of a vertex v corresponds to the sum of the entries in the row (or column) of the distance matrix $\mathcal{D}$ associated with v. The

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diagonal matrix is called the *transmission matrix*, and its i-th diagonal entry is $\mathcal{T}(\mathcal{G})_{i,i}$. The *transmission* of a vertex v_i in $\mathcal{G}$, denoted by $\mathcal{T}r(v_i)$, is defined as the sum of distances from v_i to all other vertices in $\mathcal{G}$:

$$\mathcal{T}r(v_i) = \sum_{\substack{j=1 \\ j\neq i}}^{n} d_{ij}, \tag{2}$$

The average transmission is denoted by $t(\mathcal{G})$ and is the average of the transmissions over all vertices. The average transmission for the graph $t(\mathcal{G})$, with n number of vertices, is defined as:

$$t(\mathcal{G}) = \frac{1}{n}\sum_{i=1}^{n}(\mathcal{T}r(v_i). \tag{3}$$

Let $\mathcal{A}(\mathcal{G})$ be the adjacency matrix of a graph G, and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n$ denote the eigenvalues of $\mathcal{A}(\mathcal{G})$. For convenience, we may also write $\lambda_i = \lambda_i(\mathcal{G})$.

In chemical graph theory and spectral graph analysis, distance-based matrices offer deep insights into molecular topology [2]. The *distance matrix* of $\mathcal{G}$, denoted by $\mathcal{D}(\mathcal{G}) = [d_{ij}]$, is an $n \times n$ matrix defined as follows:

$$\mathcal{D}(\mathcal{G})_{i,j} = \begin{cases} d_{ij}, & \text{if } i \neq j, \\ 0, & \text{if } i = j, \end{cases} \tag{4}$$

where d_{ij} denotes the length of the shortest path between the vertices v_i and v_j in the graph $\mathcal{G}$. The *distance spectrum* of $\mathcal{G}$ consists of all eigenvalues of the distance matrix, counted with their multiplicities. The *distance Laplacian matrix* is defined as:

$$\mathcal{DL}(\mathcal{G}) = \mathcal{T}(\mathcal{G}) - \mathcal{D}(\mathcal{G}). \tag{5}$$

The distance signless Laplacian matrix of a graph is defined as the sum of its distance matrix and the diagonal matrix of vertex transmissions. It captures both structural and spectral properties, especially in chemical graph analysis [3]. The *distance signless Laplacian matrix* is defined as:

$$\mathcal{DQ}(\mathcal{G}) = \mathcal{T}(\mathcal{G}) + \mathcal{D}(\mathcal{G}). \tag{6}$$

The distance spectrum $\mathcal{D}$-spec$(\mathcal{G})$, distance Laplacian spectrum $\mathcal{DL}$-spec$(\mathcal{G})$ and distance signless Laplacian spectrum $\mathcal{DQ}$-spec$(\mathcal{G})$ are the sets of eigenvalues of $\mathcal{D}(\mathcal{G})$, $\mathcal{DL}(\mathcal{G})$ and $\mathcal{DQ}(\mathcal{G})$, respectively, each with their corresponding multiplicities.

The study of the distance spectrum $\mathcal{D}$-spec$(\mathcal{G})$ was pioneered by Indulal and Gutman [4] in 2008. They examined the eigenvalues of the distance matrix and highlighted their role in understanding molecular symmetry, while the concepts of the distance Laplacian spectrum $\mathcal{DL}$-spec$(\mathcal{G})$ and the distance signless Laplacian spectrum $\mathcal{DQ}$-spec$(\mathcal{G})$ were introduced by Aouchiche and Hansen [5] in 2013. For further reading on distance Laplacian spectra, we refer the reader to [2,6] and the references therein. Let $n = |V(\mathcal{G})|$. The eigenvalues and the multiplicities of the distance-related matrices form the corresponding spectra:

- *$\mathcal{D}$-spectrum ($\mathcal{D}$-spec)*: The multiplicities of the eigenvalues $\{\alpha_1^{a_1}, \alpha_2^{a_2}, \ldots, \alpha_l^{a_l}\}$ of $\mathcal{D}(\mathcal{G})$.
- *$\mathcal{DL}$-spectrum ($\mathcal{DL}$-spec)*: The multiplicities of eigenvalues $\{\beta_1^{b_1}, \beta_2^{b_2}, \ldots, \beta_m^{b_m}\}$ of $\mathcal{DL}(\mathcal{G})$.
- *$\mathcal{DQ}$-spectrum ($\mathcal{DQ}$-spec)*: The multiplicities of eigenvalues $\{\gamma_1^{c_1}, \gamma_2^{c_2}, \ldots, \gamma_q^{c_q}\}$ of $\mathcal{DQ}(\mathcal{G})$.

Note that $\alpha_1, \alpha_2, \ldots, \alpha_\ell$ are the eigenvalues of $\mathcal{D}(\mathcal{G})$ with corresponding multiplicities $a_1, a_2, \ldots, a_\ell$; also, $\beta_1, \beta_2, \ldots, \beta_m$ are the eigenvalues of $\mathcal{DL}(\mathcal{G})$ with multiplicities $b_1, b_2, \ldots, b_m$; and $\gamma_1, \gamma_2, \ldots, \gamma_q$ are the eigenvalues of $\mathcal{DQ}(\mathcal{G})$ with multiplicities $c_1, c_2, \ldots, c_q$, respectively.

We can define Distance Integrality such that a connected graph $\mathcal{G}$ is called *distance integral* ($\mathcal{D}$-integral), *distance Laplacian integral* ($\mathcal{DL}$-integral), or *distance signless Laplacian integral* ($\mathcal{DQ}$-integral) if the spectrum of its respective matrix $\mathcal{D}$-spec($\mathcal{G}$), $\mathcal{DL}$-spec($\mathcal{G}$), or $\mathcal{DQ}$-spec($\mathcal{G}$) consists solely of integer eigenvalues, respectively. So, in general, we can say that a graph $\mathcal{G}$ is:

- *$\mathcal{D}$-integral* if all $\alpha_i \in \mathcal{Z}$.
- *$\mathcal{DL}$-integral* if all $\beta_i \in \mathcal{Z}$.
- *$\mathcal{DQ}$-integral* if all $\gamma_i \in \mathcal{Z}$.

The study of integral graphs began with the question, "Which graphs have integral spectra?" posed by Harary and Schwenk [7] in 1974 (see also [8,9] for more information).

Spectral methods have become central in the study of chemical graph theory, offering algebraic tools to analyze molecular structure and stability. Aouchiche and Hansen [5] introduced and investigated the spectral properties of distance Laplacian and distance signless Laplacian matrices. Their subsequent survey [10] provides extensive overviews of results and open problems in this area, covering spectral bounds, cospectrality, and extremal graphs.

The investigation of spectral integrality in molecular graphs is motivated by its close connection to fundamental structural properties of chemical compounds. Integral eigenvalues often arise in graphs exhibiting high degrees of symmetry, and such symmetry is frequently associated with enhanced molecular stability and regularity of bonding patterns [7]. In distance-based matrices, integrality of spectra may further indicate uniform distribution of interatomic distances, which is relevant for understanding molecular compactness and robustness [11]. Consequently, examining $\mathcal{D}$-, $\mathcal{DL}$-, and $\mathcal{DQ}$-integral properties is not merely a numerical exercise, but provides insight into how algebraic characteristics of molecular graphs reflect underlying chemical structure and stability, thereby strengthening the interpretative value of distance-based spectral descriptors in chemical graph theory. For a detailed exposition of developments in distance-based graph spectra, readers are referred to the comprehensive surveys by Aouchiche and Hansen [11].

In analogy to the distance energy $\mathcal{E}_{\mathcal{D}}(\mathcal{G})$, Laplacian energy $\mathcal{E}_{\mathcal{DL}}(\mathcal{G})$, and signless Laplacian energy $\mathcal{E}_{\mathcal{D}}(\mathcal{G})$ introduced by Indulal et al. [4], Gutman et al. [12], and Das et al. [3], respectively, the concepts of distance energy $\mathcal{E}_{\mathcal{D}}(\mathcal{G})$, distance Laplacian energy $\mathcal{E}_{\mathcal{DL}}(\mathcal{G})$, and distance signless Laplacian energy $\mathcal{E}_{\mathcal{DQ}}(\mathcal{G})$ were defined as follows:

The *distance energy* $\mathcal{E}_{\mathcal{D}}(\mathcal{G})$ of a graph $\mathcal{G}$ is calculated by summing the absolute values of the eigenvalues of the distance matrix of the graph and is defined as

$$\mathcal{E}_D(\mathcal{G}) = \sum_{i=1}^{n} = |\alpha_i| = \sum_{\alpha \in D\text{-spec}(G)} |\alpha| \tag{7}$$

where $\alpha_1, \alpha_2, \ldots, \alpha_n$ are the eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$.

The *distance Laplacian energy* is given by

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) = \sum_{i=1}^{n} \left| \beta_i - \frac{\text{trace}(\mathcal{DL}(\mathcal{G}))}{n} \right| = \sum_{\beta \in \mathcal{DL}\text{-spec}(\mathcal{G})} \left| \beta - \frac{\text{trace}(\mathcal{DL}(\mathcal{G}))}{n} \right| \tag{8}$$

where $\beta_1, \beta_2, \ldots, \beta_n$ are the eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ with $\mathcal{T}r(\mathcal{G})$ being the diagonal matrix of vertex transmissions.

The *distance signless Laplacian energy* is defined as

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{n} \left| \gamma_i - \frac{\text{trace}(\mathcal{DQ}(\mathcal{G}))}{n} \right| = \sum_{\gamma \in \mathcal{DQ}\text{-spec}(\mathcal{G})} \left| \gamma - \frac{\text{trace}(\mathcal{DQ}(\mathcal{G}))}{n} \right| \tag{9}$$

where $\gamma_1, \gamma_2, \ldots, \gamma_n$ are the eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G}) = \mathcal{T}r(\mathcal{G}) + \mathcal{D}(\mathcal{G})$.

As n denotes the number of vertices in the graph, the trace of a square matrix $\mathcal{A} = [a_{ij}] \in \mathbb{R}^{n\times n}$, denoted by trace$(\mathcal{A})$, is defined as the sum of its diagonal elements:

$$\text{trace}(\mathcal{A}) = \sum_{i=1}^{n} a_{ii} \tag{10}$$

In the context of chemical graph theory, the trace of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ and the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ is given by:

$$\text{trace}(\mathcal{DL}(\mathcal{G})) = \text{trace}(\mathcal{DQ}(\mathcal{G})) = \text{trace}(\mathcal{T}(\mathcal{G})) = \sum_{i=1}^{n} \mathcal{T}_{ii} \tag{11}$$

Numerous results on the distance energy $\mathcal{E}_{\mathcal{D}}(\mathcal{G})$ have been extensively investigated by various researchers (see, for example, [13–15]). In addition, several bounds for $\mathcal{E}_{\mathcal{D}}(\mathcal{G})$, $\mathcal{E}_{\mathcal{DL}}(\mathcal{G})$, and $\mathcal{E}_{\mathcal{DQ}}(\mathcal{G})$, as well as the relationships among these three energy measures, have been explored in [3,12,16] and the references therein.

Previous research in chemical graph theory has focused on developing and analyzing various topological indices and molecular descriptors, including Zagreb-type, eccentricity-based, and degree-related indices, along with their bounds and generalizations. These studies provide a solid combinatorial foundation for molecular graph analysis, while our work extends this direction by emphasizing distance-based spectral matrices and their integrality properties from a linear algebraic perspective; see [17–20] for more detail.

Together, these works form a substantial foundation in the combinatorial study of molecular graphs. The present paper complements this body of research by shifting the focus toward distance-based spectral matrices and their integrality properties from a linear algebraic perspective.

The paper is organized as follows. Section 2 details the computational methodology employed, including the construction of distance-based matrices, eigenvalue computations using NumPy and SymPy, integrality verification, energy calculations, and graphical visualizations. Following this, the results and discussions are presented, beginning with an overview of the selected molecular graphs and their objectives. Section 4 provides a detailed molecular graph analysis, examining the spectral properties, integrality, and energies for each hydrocarbon structure, such as Formaldehyde (CH_2O), Methane (CH_4), Methanol (CH_3OH), Ethylene (C_2H_4), Ethylene Glycol $(C_2H_6O_2)$, Benzene (C_6H_6), Toluene $(C_6H_5CH_3)$, and Cyclohexane (C_6H_{12}). Graphical comparisons and correlations between spectral properties and molecular structures are highlighted throughout. Finally, conclusions and potential future directions are summarized.

2. Computational Methodology

The computational procedure consists of the following steps:

1. The distance matrix $\mathcal{D}(\mathcal{G})$ for each molecular graph $\mathcal{G}$ was computed.
2. The transmission matrix $\mathcal{T}(\mathcal{G})$, the distance Laplacian matrix $\mathcal{DL}(\mathcal{G}) = \mathcal{T}(\mathcal{G}) - \mathcal{D}(\mathcal{G})$, and the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G}) = \mathcal{T}(\mathcal{G}) + \mathcal{D}(\mathcal{G})$ were constructed accordingly.
3. All numerical computations related to the construction of distance-based matrices, eigenvalue evaluation, and energy calculations were carried out using Python 3.14 In particular, the NumPy and SciPy libraries were employed for matrix operations and linear algebra computations, which were used to support and verify the analytical results presented in this work.

4. The integrality of the spectra was checked numerically by verifying whether the eigenvalues are integers or not.
5. The spectral energies, i.e., ($\mathcal{E}_{\mathcal{D}}$), ($\mathcal{E}_{\mathcal{DL}}$), and ($\mathcal{E}_{\mathcal{DQ}}$), were computed using their respective definitions. Integrality results were also tabulated.
6. To facilitate comparative analysis, the spectral energies were visualized through graphical representation.The visualization highlights structural differences and spectral behavior among the selected molecular graphs.

In the molecular structures presented in the following section, carbon, oxygen, and hydrogen atoms are depicted in magenta, red, and cyan, respectively.

3. Results and Discussions

This section reports the computed distance-based spectral properties and energies for a comprehensive set of eight molecular graphs: Methane (CH_4), Ethylene (C_2H_4), Methanol (CH_3OH), Formaldehyde (CH_2O), Benzene (C_6H_6), Ethylene Glycol ($C_2H_6O_2$), Aromatic Hydrocarbon Toluene ($C_6H_5CH_3$), and Cyclohexane (C_6H_{12}). The analysis focuses on two main objectives: first, determining the integrality of the distance matrices ($\mathcal{D}$-integral, $\mathcal{DL}$-integral, $\mathcal{DQ}$-integral), and second, conducting a comparative assessment of the calculated distance energies ($\mathcal{E}_{\mathcal{D}}$, $\mathcal{E}_{\mathcal{DL}}$, and $\mathcal{E}_{\mathcal{DQ}}$).

The study of graph matrices, such as the distance matrix, and their spectral properties provides insights into the topological and chemical properties of molecules. The distance matrix $\mathcal{D}(\mathcal{G})$, distance Laplacian $\mathcal{DL}(\mathcal{G})$, and distance signless Laplacian $\mathcal{DQ}(\mathcal{G})$ provide insights into graph structure via their eigenvalues, with integral spectra ($\mathcal{D}$-integral, $\mathcal{DL}$-integral, $\mathcal{DQ}$-integral) indicating potential symmetry or stability [21–23]. This work extends the framework of chemical graphs by analyzing their spectral properties. The work of Xu et al. [24] on extremal properties of distance-based graph invariants provides a foundation that supports the analysis of spectral properties and energies of molecular graphs in the present study. Our objectives are to:

- Determine whether chemical graphs are $\mathcal{D}$-integral, $\mathcal{DL}$-integral, or $\mathcal{DQ}$-integral.
- Compute distance energies ($\mathcal{E}_{\mathcal{D}}$, $\mathcal{E}_{\mathcal{DL}}$, $\mathcal{E}_{\mathcal{DQ}}$) and make a comparison among them.
- Explore correlations between spectral properties and molecular structures using linear algebra techniques.
- Provide graphical comparisons to highlight trends in molecular graphs.

4. Molecular Graph Analysis

To ensure clarity across all structural representations, a uniform visualization key is applied throughout the following subsections: carbon atoms are colored red, hydrogen atoms are cyan, and oxygen atoms are colored magenta. Each subsection begins by establishing the molecular graph topology, followed by the detailed construction and calculation of the distance-based matrices, their corresponding eigenvalues, and the resulting energy measures ($\mathcal{E}_{\mathcal{D}}$, $\mathcal{E}_{\mathcal{DL}}$, and $\mathcal{E}_{\mathcal{DQ}}$) for the specific molecule. All molecular graphs considered in this study correspond to organic molecules commonly used in chemical graph theory. In this work, the proposed spectral and energy analysis is restricted to molecular graphs representing single molecules, and therefore focuses exclusively on intra-molecular structures. Extensions of this framework to molecular clusters or multi-molecular systems a re beyond the scope of the present study and may be considered in future research.

4.1. Formaldehyde (CH_2O)—Simple Carbonyl Compound

Formaldehyde, denoted chemically as CH_2O, is the simplest aldehyde and consists of a carbon atom double-bonded to an oxygen atom and single-bonded to two hydrogen atoms. It is a colorless, flammable gas with a strong pungent odor and is widely used in the

production of industrial resins, disinfectants, and preservatives [25]. A *star graph* S_3, where the central vertex is the carbon atom, connected to two hydrogen atoms and one oxygen atom (double bond), is shown in Figure 1. The Laplacian matrix will help in understanding how the bonds interact and the structure of the Formaldehyde molecule.

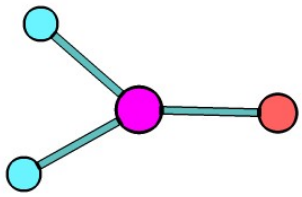

Figure 1. Formaldehyde (CH_2O).

4.2. Spectral Properties of Formaldehyde (CH_2O)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$V(\mathcal{G}) = \{v_1 = \mathrm{C},\ v_2 = \mathrm{H}_1(\text{on C}),\ v_3 = \mathrm{H}_2(\text{on C}),\ v_4 = O(\text{on to C})\}.$$

Then, the distance matrix $\mathcal{D}(\mathcal{G})$ is:

$$\mathcal{D}(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 2 & 2 \\ 1 & 2 & 0 & 2 \\ 1 & 2 & 2 & 0 \end{bmatrix}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Formaldehyde (CH_2O) are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-2]^2,\ [-0.6458]^2,\ [4.6458]^1\}.$$

The corresponding distance energy is:

$$\mathcal{E}_{\mathcal{D}}(\mathcal{G}) = \sum_{i=1}^{4} |\alpha_i| = 2 + 2 + 0.64581 + 4.6458 \approx 9.2915\ .$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-2]^2,\ [-0.6458]^2,\ [4.6458]^1\}.$$

Since not all eigenvalues are integers for Formaldehyde, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \mathrm{diag}(3, 5, 5, 5).$$

Thus, the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ is:

$$\mathcal{DL}(\mathcal{G}) = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 5 & -2 & -2 \\ -1 & -2 & 5 & -2 \\ -1 & -2 & -2 & 5 \end{bmatrix}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[0]^1,\ [4]^1,\ [7]^2\}.$$

The corresponding $\mathcal{DQ}$-energy is:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{6}\left|\gamma_i - \frac{\text{trace}(\mathcal{DQ}(\mathcal{G}))}{|V(G)|}\right|.$$

Given that $\text{trace}(DL(\mathcal{G})) = 18$, and $n = 4$, the average is $\frac{18}{4} = 4.5$, so:

$$\begin{aligned}\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) &= \sum_{i=1}^{6}\left|\beta_i - \frac{\text{trace}(\mathcal{DL}(\mathcal{G}))}{n}\right|,\\ &= \sum_{i=1}^{6}|\beta_i - 4.5| \approx 10.0\end{aligned}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{0,\ 4,\ 7,\ 7\}.$$

Since all eigenvalues are integers for Formaldehyde, we conclude that $\mathcal{G}$ is $\mathcal{DL}$-integral.

The distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ is:

$$\mathcal{DQ}(\mathcal{G}) = \begin{bmatrix}3 & 1 & 1 & 1\\ 1 & 5 & 2 & 2\\ 1 & 2 & 5 & 2\\ 1 & 2 & 2 & 5\end{bmatrix}$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[2.5359]^1,\ [3]^2,\ [9.4641]^2\}.$$

Given that $\text{trace}(\mathcal{DQ}(\mathcal{G})) = 18$, and $n = 4$, the average is again $\frac{18}{4} \approx 4.5$, so:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{4}\left|\gamma_i - \frac{\text{trace}(\mathcal{DQ}(\mathcal{G}))}{5}\right| = \sum_{i=1}^{4}|\gamma_i - 4.5| \approx 9.9282.$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[2.5359]^1,\ [3]^2,\ [9.4641]^2\}.$$

Since not all eigenvalues are integers for Formaldehyde, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

4.3. Methane (CH_4)—Tetrahedral Structure

The molecular structure of methane consists of a carbon atom which is bonded to four hydrogen atoms in a tetrahedral shape. So, the graph of Methane consists of 5 vertices and 4 edges, where vertices represent atoms and edges represent covalent bonds; see Figure 2.

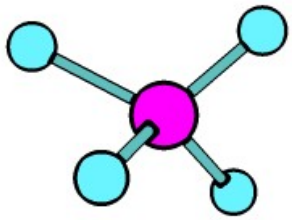

Figure 2. Methane (CH_4).

4.4. Spectral Properties of Methane (CH_4)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$V(\mathcal{G}) = \{v_1 = \mathrm{C},\ v_2 = \mathrm{H}_1(\text{on C}),\ v_3 = \mathrm{H}_2(\text{on C}),\ v_4 = \mathrm{H}_3(\text{on C}), v_5 = \mathrm{H}_4(\text{on C}\}.$$

The distance matrix $\mathcal{D}(\mathcal{G})$ is:

$$\mathcal{D}(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 2 & 2 & 2 \\ 1 & 2 & 0 & 2 & 2 \\ 1 & 2 & 2 & 0 & 2 \\ 1 & 2 & 2 & 2 & 0 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of methane (CH_4) form the distance spectrum, denoted by $\mathcal{D}$-spec$(\mathcal{G})$. These values are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) &= \{-2,\ -2,\ -2,\ -0.6056,\ 6.6056\} \\ &= \{[-2]^3,\ [-0.6056]^1,\ [6.6056]^1\}. \end{aligned}$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) &= \sum_{i=1}^{5} |\alpha_i| = 3|-2| + |-0.6056| + |6.6056| \\ &= 13.2112 \approx 13.21\ . \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-2]^3,\ [-0.6056]^1,\ [6.6056]^1\}.$$

Since not all eigenvalues are integers for Methane, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \mathrm{diag}(4,7,7,7,7),$$

$$\mathcal{DL}(\mathcal{G}) = \begin{bmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 7 & -2 & -2 & -2 \\ -1 & -2 & 7 & -2 & -2 \\ -1 & -2 & -2 & 7 & -2 \\ -1 & -2 & -2 & -2 & 7 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DL}\text{-spec}(\mathcal{G}) &= \{0,\ 5,\ 9,\ 9,\ 9\},\\ &= \{[0]^1,\ [5]^1,\ [9]^3\}.\end{aligned}$$

Given that $\text{tr}(\mathcal{DL}(\mathcal{G})) = 32$, and $n = 5$, the average is $\frac{32}{5} \approx 6.4$, and the corresponding $\mathcal{DL}$-energy is given by:

$$\begin{aligned}\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) &= \sum_{i=1}^{5} |\beta_i - 6.4| = |0 - 6.4| + |5 - 6.4| + 3 \times |9 - 6.4|,\\ &= 6.4 + 1.4 + 3 \times 2.6 = 6.4 + 1.4 + 7.8 = 15.60\ .\end{aligned}$$

The eigenvalues (with their corresponding multiplicities) of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[0]^1,\ [5]^1,\ [9]^3\}.$$

Since all eigenvalues are integers for Methane, we conclude that $\mathcal{G}$ is $\mathcal{DL}$-integral. The distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ is:

$$\mathcal{DQ}(\mathcal{G}) = \begin{bmatrix} 4 & 1 & 1 & 1 & 1 \\ 1 & 7 & 2 & 2 & 2 \\ 1 & 2 & 7 & 2 & 2 \\ 1 & 2 & 2 & 7 & 2 \\ 1 & 2 & 2 & 2 & 7 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DQ}\text{-spec}(\mathcal{G}) &= \{3.5756,\ 5,\ 5,\ 5,\ 13.4244\},\\ &= \{3.5756^{[1]},\ 5^{[3]},\ 13.4244^{[1]}\}.\end{aligned}$$

The corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{5} \left| \gamma_i - \frac{\text{trace}(DQ(\mathcal{G}))}{|V(G)|} \right|.$$

Given that $\text{trace}(DQ(\mathcal{G})) = 32$, and $n = 5$, the average is again $\frac{32}{5} \approx 6.4$, so:

$$\begin{aligned}\mathcal{E}_{DQ}(\mathcal{G}) &= \sum_{i=1}^{5} \left| \gamma_i - \frac{32}{5} \right| = |3.5756 - 6.4| + 3 \times |5 - 6.4| + |13.4244 - 6.4|,\\ &= 2.8244 + 3 \times 1.4 + 7.0244 = 2.8244 + 4.2 + 7.0244 = 14.05\ .\end{aligned}$$

The eigenvalues (with their corresponding multiplicities) of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[5]^1,\ [6.5538]^1,\ [8]^1,\ [9]^2,\ [20.4462]^1\}.$$

Since not all eigenvalues are integers for Methane, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

4.5. Methanol (CH_3OH)—Alcohol Group

In chemical graph theory, methanol is represented as a tree graph consisting of 6 vertices representing atoms: one carbon (C), one oxygen (O), and four hydrogens (H). The carbon atom has degree four, connected to three hydrogen atoms and one oxygen atom. The oxygen atom has degree two, bonded to the carbon and one hydrogen atom. The resulting molecular graph is connected and models the topology of methanol as a simple labeled graph without cycles that reflects the valency; see Figure 3.

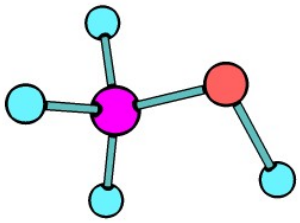

Figure 3. Methanol (CH_3OH).

4.6. Spectral Properties of Methanol (CH_3OH)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$\begin{aligned} V(\mathcal{G}) =& \{v_1 = \mathrm{C},\ v_2 = \mathrm{H}_1(\text{on C}),\ v_3 = \mathrm{H}_2(\text{on C}),\ v_4 = \mathrm{H}_3(\text{on C}),\ v_5 = \mathrm{H}_4(\text{on C}),\\ & v_6 = \mathrm{O}(\text{on to H}_4)\}. \end{aligned}$$

Then, the distance matrix $\mathcal{D}(\mathcal{G})$ is:

$$\mathcal{D}(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 2 \\ 1 & 0 & 2 & 2 & 2 & 3 \\ 1 & 2 & 0 & 2 & 2 & 3 \\ 1 & 2 & 2 & 0 & 2 & 3 \\ 1 & 2 & 2 & 2 & 0 & 1 \\ 2 & 3 & 3 & 3 & 1 & 0 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Methanol (CH_3OH) are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-4.1409]^1,\ [-2]^2,\ [-1.0566]^1,\ [-0.4727]^1,\ [9.6702]^1\}.$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) &= \sum_{i=1}^{6} |\alpha_i|, \\ &= 4.1409 + 2 + 2 + 1.0566 + 0.4727 + 9.6702 \\ &= 19.3404\ . \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-4.1409]^1,\ [-2]^2,\ [-1.0566]^1,\ [-0.4727]^1,\ [9.6702]^1\}.$$

Since not all eigenvalues are integers for Methanol, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \mathrm{diag}(6, 10, 10, 10, 8, 12).$$

Thus, the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ is:

$$\mathcal{DL}(\mathcal{G}) = \begin{bmatrix} 6 & -1 & -1 & -1 & -1 & -2 \\ -1 & 10 & -2 & -2 & -2 & -3 \\ -1 & -2 & 10 & -2 & -2 & -3 \\ -1 & -2 & -2 & 10 & -2 & -3 \\ -1 & -2 & -2 & -2 & 8 & -1 \\ -2 & -3 & -3 & -3 & -1 & 12 \end{bmatrix}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[-0]^1,\ [7.0444]^1,\ [9.7405]^1,\ [12]^2,\ [15.2151]^1\}.$$

Given that $\text{trace}(\mathcal{DL}(\mathcal{G})) = 56$, and $n = 6$, the average is $\frac{56}{6} \approx 9.3333$, so the corresponding $\mathcal{DL}$-energy is given by:

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) = \sum_{i=1}^{6} \left| \beta_i - \frac{\text{trace}(\mathcal{DL}(\mathcal{G}))}{n} \right| = \sum_{i=1}^{6} \left| \beta_i - \frac{56}{6} \right| \approx 23.2445.$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[-0]^1,\ [7.0444]^1,\ [9.7405]^1,\ [12]^2,\ [15.2151]^1\}.$$

Since all eigenvalues are not integers for Methanol, we conclude that $\mathcal{G}$ is not $\mathcal{DL}$-integral.

$$\mathcal{DQ}(\mathcal{G}) = \begin{bmatrix} 6 & 1 & 1 & 1 & 1 & 2 \\ 1 & 10 & 2 & 2 & 2 & 3 \\ 1 & 2 & 10 & 2 & 2 & 3 \\ 1 & 2 & 2 & 10 & 2 & 3 \\ 1 & 2 & 2 & 2 & 8 & 1 \\ 2 & 3 & 3 & 3 & 1 & 12 \end{bmatrix}$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[5.1290]^1,\ [6.2370]^1,\ [8]^2,\ [8.8015]^1,\ [19.8325]^1\}.$$

Given that $\text{trace}(\mathcal{DQ}(\mathcal{G})) = 56$, and $n = 6$, the average is again $\frac{56}{6} \approx 9.3333$, so the corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{6} \left| \gamma_i - \frac{\text{trace}(\mathcal{DQ}(\mathcal{G}))}{6} \right| = \sum_{i=1}^{6} |\gamma_i - 9.3333| \approx 20.9983.$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[5.1290]^1,\ [6.2370]^1,\ [8]^2,\ [8.8015]^1,\ [19.8325]^1\}.$$

Since not all eigenvalues are integers for Methanol, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

4.7. Ethylene (C_2H_4)—Planar Double Bond

Ethylene, also known as ethylene, is a simple hydrocarbon with the molecular formula C_2H_4. In chemical graph theory, Ethylene can be represented as an molecular graph, where vertices correspond to atoms and edges to covalent bonds. Each carbon atom is a vertex with degree 3. Each hydrogen atom is a vertex with degree 1. It is represented as a planar

graph with two carbon atoms connected by a double bond, and each carbon atom bonded to two hydrogen atoms; see Figure 4.

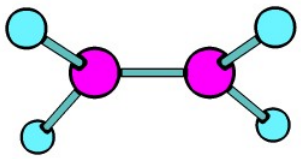

Figure 4. Ethylene (C_2H_4).

4.8. Spectral Properties of Ethylene (C_2H_4)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$\begin{aligned} V(\mathcal{G}) =& \{v_1 = \mathrm{C}_1,\ v_2 = \mathrm{C}_2,\ v_3 = \mathrm{H}_1(\text{on } \mathrm{C}_1),\ v_4 = \mathrm{H}_2(\text{on } \mathrm{C}_1),\ v_5 = \mathrm{H}_3(\text{on } \mathrm{C}_2), \\ & v_6 = \mathrm{H}_4(\text{on } \mathrm{C}_2)\}. \end{aligned}$$

Then, the distance matrix $\mathcal{D}(\mathcal{G})$ is:

$$\mathcal{D}(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 1 & 1 & 2 & 2 \\ 1 & 0 & 2 & 2 & 1 & 1 \\ 1 & 2 & 0 & 2 & 3 & 3 \\ 1 & 2 & 2 & 0 & 3 & 3 \\ 2 & 1 & 3 & 3 & 0 & 2 \\ 2 & 1 & 3 & 3 & 2 & 0 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Ethylene (C_2H_4) are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-4.5616]^1,\ [-2]^2,\ [-1]^1,\ [-0.4384]^1,\ [10]^1\}.$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) &= \sum_{i=1}^{6} |\alpha_i| = |-4.5616| + |-2| + |-2| + |-1| + |-0.4384| + |10| \\ &= 19.9999. \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\mathcal{D}\text{-spec}(\mathcal{G}) = \{[-4.5616]^1,\ [-2]^2,\ [-1]^1,\ [-0.4384]^1,\ [10]^1\}.$$

Not all eigenvalues for Ethylene in $\mathcal{D}$-spec, are integers. So, $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \mathrm{diag}(7, 7, 11, 11, 11, 11).$$

Thus, the distance Laplacian matrix is:

$$\mathcal{DL}(\mathcal{G}) = \begin{bmatrix} 7 & -1 & -1 & -1 & -2 & -2 \\ -1 & 7 & -2 & -2 & -1 & -1 \\ -1 & -2 & 11 & -2 & -3 & -3 \\ -1 & -2 & -2 & 11 & -3 & -3 \\ -2 & -1 & -3 & -3 & 11 & -2 \\ -2 & -1 & -3 & -3 & -2 & 11 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[0]^1,\ [7.7251]^1,\ [9]^1,\ [13]^2,\ [15.2749]^1\}.$$

Given that $\text{trace}(\mathcal{DL}(\mathcal{G})) = 58$, and $n = 6$, the average is $\frac{58}{6} \approx 9.6667$, so the corresponding Distance Laplacian energy $\mathcal{DL}$-energy is given by:

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) = \sum_{i=1}^{6} |\beta_i - 9.6667| \approx 24.5498.$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[0]^1,\ [7.7251]^1,\ [9]^1,\ [13]^2,\ [15.2749]^1\}.$$

For Ethylene, not all eigenvalues in $\mathcal{DL}$-spec integers. So, we conclude that $\mathcal{G}$ is not $\mathcal{DL}$-integral. Thus, the distance Signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ is:

$$\mathcal{DQ}(\mathcal{G}) = \begin{bmatrix} 7 & 1 & 1 & 1 & 2 & 2 \\ 1 & 7 & 2 & 2 & 1 & 1 \\ 1 & 2 & 11 & 2 & 3 & 3 \\ 1 & 2 & 2 & 11 & 3 & 3 \\ 2 & 1 & 3 & 3 & 11 & 2 \\ 2 & 1 & 3 & 3 & 2 & 11 \end{bmatrix}$$

The eigenvalues (with their corresponding multiplicities) of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[5]^1,\ [6.5538]^1,\ [8]^1,\ [9]^2,\ [20.4462]^1\}.$$

Given that $\text{trace}(\mathcal{DQ}(\mathcal{G})) = 58$, and $n = 6$, the average is again $\frac{58}{6} \approx 9.6667$, so the corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{6} |\gamma_i - 9.6667| = 21.5592 \approx 21.56\ .$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[5]^1,\ [6.5538]^1,\ [8]^1,\ [9]^2,\ [20.4462]^1\}.$$

Since not all eigenvalues in $\mathcal{DQ}$-spec are integers for Ethylene, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral. Since not all eigenvalues in $\mathcal{D}$-spec, $\mathcal{DL}$-spec, or $\mathcal{DQ}$-spec are integers, the graph of Ethylene is neither $\mathcal{D}$-integral, $\mathcal{DL}$-integral, nor $\mathcal{DQ}$-integral.

4.9. Ethylene Glycol ($C_2H_6O_2$)—Diol Structure

In chemical graph theory, ethylene glycol ($C_2H_6O_2$), also known as ethane-1,2-diol, is represented as a molecular graph with ten vertices: two carbon atoms (C), two oxygen atoms (O), and six hydrogen atoms (H); see Figure 5. Each carbon atom is connected to two hydrogen atoms and one oxygen atom; the two carbon atoms are also bonded to each other, forming the backbone of the molecule. Each oxygen atom is additionally bonded to one hydrogen atom. The resulting molecular graph is undirected, connected, acyclic (a tree), and satisfies the valency constraints of all constituent atoms. Ethylene glycol is the simplest example of a *diol*, containing two hydroxyl groups.

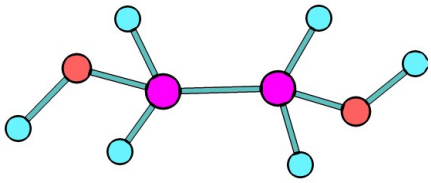

Figure 5. Ethylene Glycol $(C_2H_6O_2)$.

4.10. Spectral Properties of Ethylene Glycol ($C_2H_6O_2$)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$\begin{aligned} V(\mathcal{G}) =& \{v_1 = \mathrm{C}_1, v_2 = \mathrm{C}_2, v_3 = \mathrm{H}_1(\text{on } \mathrm{C}_1), v_4 = \mathrm{H}_2(\text{on } \mathrm{C}_1), v_5 = \mathrm{H}_3(\text{on } \mathrm{C}_2), v_6 = \mathrm{H}_4 \\ & (\text{on } \mathrm{C}_2), v_7 = \mathrm{O}_1(\text{on } \mathrm{C}_1), v_8 = \mathrm{O}_2(\text{on } \mathrm{C}_2), v_9 = \mathrm{H}_5(\text{on } \mathrm{O}_1), v_{10} = \mathrm{H}_6(\text{on } \mathrm{O}_2)\}. \end{aligned}$$

Then, the distance matrix $\mathcal{D}(\mathcal{G})$ is:

$$\mathcal{D}(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 1 & 1 & 2 & 2 & 1 & 2 & 2 & 3 \\ 1 & 0 & 2 & 2 & 1 & 1 & 2 & 1 & 3 & 2 \\ 1 & 2 & 0 & 2 & 3 & 3 & 2 & 3 & 3 & 4 \\ 1 & 2 & 2 & 0 & 3 & 3 & 2 & 3 & 3 & 4 \\ 2 & 1 & 3 & 3 & 0 & 2 & 3 & 2 & 4 & 3 \\ 2 & 1 & 3 & 3 & 2 & 0 & 3 & 2 & 4 & 3 \\ 1 & 2 & 2 & 2 & 3 & 3 & 0 & 3 & 1 & 4 \\ 2 & 1 & 3 & 3 & 2 & 2 & 3 & 0 & 4 & 1 \\ 2 & 3 & 3 & 3 & 4 & 4 & 1 & 4 & 0 & 5 \\ 3 & 2 & 4 & 4 & 3 & 3 & 4 & 1 & 5 & 0 \end{bmatrix}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Ethylene Glycol $(C_2H_6O_2)$ are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-8.5823]^1,\ [-4.098]^1,\ [-3.248]^1,\ [-2]^2,\ [-1.3655]^1,\ [-0.8194]^1, \\ &[-0.5589]^1,\ [-0.3502]^1,\ [23.0224]^1\}. \end{aligned}$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) = \sum_{i=1}^{10} |\alpha_i| &= |-8.5823| + |-4.098| + |-3.248| + |-2| + |-2| + |-1.3655| \\ &+ |-0.8194| + |-0.5589| + |-0.3502| + |23.0224| \approx 46.0447\ . \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-8.5823]^1,\ [-4.098]^1,\ [-3.248]^1,\ [-2]^2,\\ &[-1.3655]^1,\ [-0.8194]^1,\ [-0.5589]^1,\ [-0.3502]^1,\ [23.0224]^1\}.\end{aligned}$$

Since not all eigenvalues are integers for Ethylene Glycol, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \text{diag}(15, 15, 23, 23, 23, 23, 21, 21, 29, 29).$$

The distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ is:

$$\mathcal{DL}(\mathcal{G}) = \begin{bmatrix} 15 & -1 & -1 & -1 & -2 & -2 & -1 & -2 & -2 & -3 \\ -1 & 15 & -2 & -2 & -1 & -1 & -2 & -1 & -3 & -2 \\ -1 & -2 & 23 & -2 & -3 & -3 & -2 & -3 & -3 & -4 \\ -1 & -2 & -2 & 23 & -3 & -3 & -2 & -3 & -3 & -4 \\ -2 & -1 & -3 & -3 & 23 & -2 & -3 & -2 & -4 & -3 \\ -2 & -1 & -3 & -3 & -2 & 23 & -3 & -2 & -4 & -3 \\ -1 & -2 & -2 & -2 & -3 & -3 & 21 & -3 & -1 & -4 \\ -2 & -1 & -3 & -3 & -2 & -2 & -3 & 21 & -4 & -1 \\ -2 & -3 & -3 & -3 & -4 & -4 & -1 & -4 & 29 & -5 \\ -3 & -2 & -4 & -4 & -3 & -3 & -4 & -1 & -5 & 29 \end{bmatrix}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DL}\text{-spec}(\mathcal{G}) = \{&[0]^1,\ [15.7223]^1,\ [17.1899]^1,\ [22.9334]^1,\ [23.1805]^1,\ [25]^2,\\ &[27.021]^1,\ [30.6296]^1,\ [35.3233]^1\}.\end{aligned}$$

Given that $\text{trace}(\mathcal{DL}(\mathcal{G})) = 222$, and $n = 10$, the average is $\frac{222}{10} \approx 22.2$, so the corresponding $\mathcal{DL}$-energy is given by:

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) = \sum_{i=1}^{12} |\beta_i - 22.2| \approx 67.3755.$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DL}\text{-spec}(\mathcal{G}) = \{&[0]^1,\ [15.7223]^1,\ [17.1899]^1,\ [22.9334]^1,\ [23.1805]^1, [25]^2,\\ &[27.021]^1,\ [30.6296]^1,\ [35.3233]^1\}.\end{aligned}$$

Since not all eigenvalues are integers for Ethylene Glycol, we conclude that $\mathcal{G}$ is not $\mathcal{DL}$-integral. The distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ is:

$$\mathcal{DQ}(\mathcal{G}) = \begin{bmatrix} 15 & 1 & 1 & 1 & 2 & 2 & 1 & 2 & 2 & 3 \\ 1 & 15 & 2 & 2 & 1 & 1 & 2 & 1 & 3 & 2 \\ 1 & 2 & 23 & 2 & 3 & 3 & 2 & 3 & 3 & 4 \\ 1 & 2 & 2 & 23 & 3 & 3 & 2 & 3 & 3 & 4 \\ 2 & 1 & 3 & 3 & 23 & 2 & 3 & 2 & 4 & 3 \\ 2 & 1 & 3 & 3 & 2 & 23 & 3 & 2 & 4 & 3 \\ 1 & 2 & 2 & 2 & 3 & 3 & 21 & 3 & 1 & 4 \\ 2 & 1 & 3 & 3 & 2 & 2 & 3 & 21 & 4 & 1 \\ 2 & 3 & 3 & 3 & 4 & 4 & 1 & 4 & 29 & 5 \\ 3 & 2 & 4 & 4 & 3 & 3 & 4 & 1 & 5 & 29 \end{bmatrix}$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[12.7609]^1,\ [14.307]^1,\ [16.851]^1,\ [19.518]^1,\ [20.0328]^1,\ [21]^2,\ [23.7465]^1,\ [25.3553]^1,\ [47.4285]^1\}.$$

Given that $\text{trace}(\mathcal{DQ}(\mathcal{G})) = 222$, and $n = 10$, the average is again $\frac{222}{12} \approx 22.2$, so the corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{10} |\gamma_i - 22.2| \approx 59.8605.$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = [21]^2,\ [23.7465]^1,\ [25.3553]^1,\ [47.4285]^1\}.$$

Since not all eigenvalues are integers for Ethylene Glycol, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

4.11. Benzene (C_6H_6)—Aromatic Ring

A cycle graph C_6, similar to cyclohexane but with alternating single and double bonds between the carbon atoms. Benzene (C_6H_6) is an aromatic hydrocarbon represented in chemical graph theory as a planar, cyclic molecular graph with six carbon atoms forming a cycle graph C_6; see Figure 6. Each carbon is bonded to one hydrogen atom, and alternating single and double bonds form a conjugated π-electron system. Benzene's conjugated π-electron system and aromatic stability can be modeled using this graph. Each vertex represents a carbon atom, and edges represent bonds. The Laplacian and signless Laplacian matrices for benzene will provide information about its resonance and symmetry.

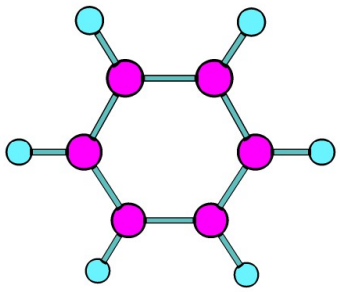

Figure 6. Benzene (C_6H_6).

4.12. Spectral Properties of Benzene (C_6H_6)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$V(\mathcal{G}) = \{v_1 = \text{C}_1,\ v_2 = \text{C}_2,\ v_3 = \text{C}_3,\ v_4 = \text{C}_4,\ v_5 = \text{C}_5,\ v_6 = \text{C}_6, v_7 = \text{H}_1(\text{on C}_1),\ v_8 = \text{H}_2(\text{on C}_2),\ v_9 = \text{H}_3(\text{on C}_3),\ v_{10} = \text{H}_4(\text{on C}_4),\ v_{11} = \text{H}_5(\text{on C}_5),\ v_{12} = \text{H}_6(\text{on C}_6)\}.$$

The distance matrix $\mathcal{D}(\mathcal{G})$ is:

$$\mathcal{D}(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 & 1 & 2 & 3 & 4 & 3 & 2 \\ 1 & 0 & 1 & 2 & 3 & 2 & 2 & 1 & 2 & 3 & 4 & 3 \\ 2 & 1 & 0 & 1 & 2 & 3 & 3 & 2 & 1 & 2 & 3 & 4 \\ 3 & 2 & 1 & 0 & 1 & 2 & 4 & 3 & 2 & 1 & 2 & 3 \\ 2 & 3 & 2 & 1 & 0 & 1 & 3 & 4 & 3 & 2 & 1 & 2 \\ 1 & 2 & 3 & 2 & 1 & 0 & 2 & 3 & 4 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 0 & 3 & 4 & 5 & 4 & 3 \\ 2 & 1 & 2 & 3 & 4 & 3 & 3 & 0 & 3 & 4 & 5 & 4 \\ 3 & 2 & 1 & 2 & 3 & 4 & 4 & 3 & 0 & 3 & 4 & 5 \\ 4 & 3 & 2 & 1 & 2 & 3 & 5 & 4 & 3 & 0 & 3 & 4 \\ 3 & 4 & 3 & 2 & 1 & 2 & 4 & 5 & 4 & 3 & 0 & 3 \\ 2 & 3 & 4 & 3 & 2 & 1 & 3 & 4 & 5 & 4 & 3 & 0 \end{bmatrix}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Benzene (C_6H_6) are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&-9.1231,\ -9.1231,\ -3.4142,\ -2,\ -2,\ -1.8114,\ -0.8769,\ -0.8769,\\ &-0.5858, -0,\ -0,\ 29.8114\},\\ = \{&[-9.1231]^2,\ [-3.4142]^1,\ [-2]^2,\ [-1.8114]^1,\ [-0.8769]^2,\ [-0.5858]^1,\\ &[-0]^2,\ [29.8114]^1\}. \end{aligned}$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) = \sum_{i=1}^{12} |\alpha_i| &= 9.1231 + 9.1231 + 3.4142 + 2 + 2 + 1.8114 + 0.8769 + 0.8769\\ &+ 0.5858 + 0 + 0 + 29.8114 \approx 59.6228\ . \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-9.1231]^2,\ [-3.4142]^1,\ [-2]^2, [-1.8114]^1,\ [-0.8769]^2,\ [-0.5858]^1,\\ &[0]^2,\ [29.8114]^1.\} \end{aligned}$$

Since not all eigenvalues are integers for Benzene, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \text{diag}(24, 24, 24, 24, 24, 24, 34, 34, 34, 34, 34, 34).$$

Thus, the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ is:

$$\mathcal{DL}(\mathcal{G}) = \begin{bmatrix} 24 & -1 & -2 & -3 & -2 & -1 & -1 & -2 & -3 & -4 & -3 & -2 \\ -1 & 24 & -1 & -2 & -3 & -2 & -2 & -1 & -2 & -3 & -4 & -3 \\ -2 & -1 & 24 & -1 & -2 & -3 & -3 & -2 & -1 & -2 & -3 & -4 \\ -3 & -2 & -1 & 24 & -1 & -2 & -4 & -3 & -2 & -1 & -2 & -3 \\ -2 & -3 & -2 & -1 & 24 & -1 & -3 & -4 & -3 & -2 & -1 & -2 \\ -1 & -2 & -3 & -2 & -1 & 24 & -2 & -3 & -4 & -3 & -2 & -1 \\ -1 & -2 & -3 & -4 & -3 & -2 & 34 & -3 & -4 & -5 & -4 & -3 \\ -2 & -1 & -2 & -3 & -4 & -3 & -3 & 34 & -3 & -4 & -5 & -4 \\ -3 & -2 & -1 & -2 & -3 & -4 & -4 & -3 & 34 & -3 & -4 & -5 \\ -4 & -3 & -2 & -1 & -2 & -3 & -5 & -4 & -3 & 34 & -3 & -4 \\ -3 & -4 & -3 & -2 & -1 & -2 & -4 & -5 & -4 & -3 & 34 & -3 \\ -2 & -3 & -4 & -3 & -2 & -1 & -3 & -4 & -5 & -4 & -3 & 34 \end{bmatrix}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[0]^1,\ [24]^2,\ [24.9172]^1,\ [26.7889]^2,\ [30]^1,\ [36]^2,\ [37.0828]^1,\ [41.2111]^2\}.$$

Given that $\text{trace}(\mathcal{DL}(\mathcal{G})) = 348$, and $n = 12$, the average is $\frac{348}{12} \approx 29$, so the corresponding $\mathcal{DL}$-energy is given by:

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) = \sum_{i=1}^{12} |\beta_i - 29| \approx 95.0099.$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\mathcal{DL}\text{-spec}(\mathcal{G}) = \{[0]^1,\ [24]^2,\ [24.9172]^1,\ [26.7889]^2,\ [30]^1,\ [36]^2,\ [37.0828]^1,\ [41.2111]^2\}.$$

Since not all eigenvalues are integers for Benzene, we conclude that $\mathcal{G}$ is not $\mathcal{DL}$-integral. The distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$is:

$$\mathcal{DQ}(\mathcal{G}) = \begin{bmatrix} 24 & 1 & 2 & 3 & 2 & 1 & 1 & 2 & 3 & 4 & 3 & 2 \\ 1 & 24 & 1 & 2 & 3 & 2 & 2 & 1 & 2 & 3 & 4 & 3 \\ 2 & 1 & 24 & 1 & 2 & 3 & 3 & 2 & 1 & 2 & 3 & 4 \\ 3 & 2 & 1 & 24 & 1 & 2 & 4 & 3 & 2 & 1 & 2 & 3 \\ 2 & 3 & 2 & 1 & 24 & 1 & 3 & 4 & 3 & 2 & 1 & 2 \\ 1 & 2 & 3 & 2 & 1 & 24 & 2 & 3 & 4 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 34 & 3 & 4 & 5 & 4 & 3 \\ 2 & 1 & 2 & 3 & 4 & 3 & 3 & 34 & 3 & 4 & 5 & 4 \\ 3 & 2 & 1 & 2 & 3 & 4 & 4 & 3 & 34 & 3 & 4 & 5 \\ 4 & 3 & 2 & 1 & 2 & 3 & 5 & 4 & 3 & 34 & 3 & 4 \\ 3 & 4 & 3 & 2 & 1 & 2 & 4 & 5 & 4 & 3 & 34 & 3 \\ 2 & 3 & 4 & 3 & 2 & 1 & 3 & 4 & 5 & 4 & 3 & 34 \end{bmatrix}$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[18.3431]^2,\ [22.8769]^1,\ [24]^2,\ [24.9722]^1,\ [29.6569]^2,\ [31.1231]^1,\ [32]^2,\ [61.0278]^1\}.$$

Given that $\text{trace}(\mathcal{DQ}(\mathcal{G})) = 348$, and $n = 12$, the average is again $\frac{348}{12} \approx 29$, so the corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{12} |\gamma_i - 29| \approx 82.9291.$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{[18.3431]^2,\ [22.8769]^1,\ [24]^2,\ [24.9722]^1,\ [29.6569]^2,\ [31.1231]^1,\ [32]^2,\ [61.0278]^1\}.$$

Since not all eigenvalues are integers for Benzene, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

4.13. Aromatic Hydrocarbon—Toluene ($C_6H_5CH_3$)

Toluene ($C_6H_5CH_3$) is represented in chemical graph theory as a molecular graph with 15 vertices, corresponding to all atoms: 7 carbon atoms and 8 hydrogen atoms. The structure

includes a six-membered hexagonal ring (a 6-cycle, C_6) in which each vertex represents a carbon atom. One of these ring carbon vertices is connected to an additional terminal carbon vertex that forms the methyl group (CH_3), with this terminal carbon bonded to three hydrogen atoms. The remaining five hydrogen atoms are attached singly to the other ring carbon atoms to satisfy valency (see Figure 7). The resulting graph is connected, planar, and reflects the delocalized π-electron system characteristic of aromatic hydrocarbons such as toluene.

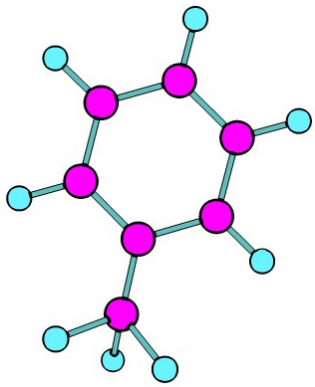

Figure 7. Toluene ($C_6H_5CH_3$).

4.14. Spectral Properties of Toluene ($C_6H_5CH_3$)

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$\begin{aligned} V(\mathcal{G}) = \{&v_1 = \mathrm{C}_1,\ v_2 = \mathrm{C}_2,\ v_3 = \mathrm{C}_3,\ v_4 = \mathrm{C}_4,\ v_5 = \mathrm{C}_5,\ v_6 = \mathrm{C}_6,\ v_7 = \mathrm{H}_1\ (\text{on } \mathrm{C}_2),\\ &v_8 = \mathrm{H}_2\ (\text{on } \mathrm{C}_3), v_9 = \mathrm{H}_3\ (\text{on } \mathrm{C}_4),\ v_{10} = \mathrm{H}_4\ (\text{on } \mathrm{C}_5),\ v_{11} = \mathrm{H}_5\ (\text{on } \mathrm{C}_6),\\ &v_{12} = \mathrm{C}_7\ (\text{on } \mathrm{C}_1),\ v_{13} = \mathrm{H}_6\ (\text{on } \mathrm{C}_7),\ v_{14} = \mathrm{H}_7\ (\text{on } \mathrm{C}_7),\ v_{15} = \mathrm{H}_8\ (\text{on } \mathrm{C}_7)\}. \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Toluene ($C_6H_5CH_3$) are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-15.9992]^1,\ [-9.1231]^1,\ [-4.8837]^1,\ [-2.85]^1,\ [-2]^3,\ [-1.8919]^1\\ &,\ [-0.9638]^1,\ [-0.8769]^1,\ [-0.6041]^1,\ [-0.4306]^1,\ [0]^2,\ [43.6233]^1\}. \end{aligned}$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) = \sum_{i=1}^{5} |\alpha_i| &= |-15.9992| + |-9.1231| + |-4.8837| + |-2.85| + |-2|\\ &+ |-2| + |-2| + |-1.8919| + |-0.9638| + |-0.8769| + |-0.6041|\\ &+ |-0.4306| + |0| + |0| + |43.6233|\\ &\approx 87.2467\ . \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-15.9992]^1,\ [-9.1231]^1,\ [-4.8837]^1,\ [-2.85]^1,\ [-2]^3,\\ &[-1.8919]^1,\ [-0.9638]^1,\ [-0.8769]^1,\ [-0.6041]^1,\ [-0.4306]^1,\\ &[0]^2,\ [43.6233]^1\}. \end{aligned}$$

Since not all eigenvalues are integers for Toluene, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \text{diag}(30, 33, 36, 39, 36, 33, 46, 49, 52, 49, 46, 37, 50, 50, 50).$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DL}\text{-spec}(\mathcal{G}) = \{&[-0]^1,\ [31.2258]^1,\ [33.9038]^1,\ [35.634]^1,\ [37.7405]^1,\ [38.078]^1,\ [40.063]^1,\\ &[43.3156]^1,\ [49.1193]^1,\ [50.9643]^1,\ [52]^2,\ [53.1883]^1,\ [54.899]^1,\ [63.8684]^1\}.\end{aligned}$$

Given that $\text{trace}(\mathcal{DL}(\mathcal{G})) = 636$, and $n = 15$, the average is $\frac{636}{15} \approx 42.4$, so the corresponding $\mathcal{DL}$-energy is given by:

$$\begin{aligned}\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) &= \sum_{i=1}^{15}\left|\beta_i - \frac{\text{trace}(\mathcal{DL}(\mathcal{G}))}{n}\right|,\\ &= \sum_{i=1}^{15}\left|\beta_i - \frac{636}{15}\right| = \sum_{i=1}^{15}|\beta_i - 42.4| \approx 160.3099.\end{aligned}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DL}\text{-spec}(\mathcal{G}) = \{&[0]^1,\ [31.2258]^1,\ [33.9038]^1,\ [35.634]^1,\ [37.7405]^1,\ [38.078]^1,[40.063]^1,\\ &[43.3156]^1,\ [49.1193]^1,\ [50.9643]^1,\ [52]^2,[53.1883]^1,\ [54.899]^1,\ [63.8684]^1\}.\end{aligned}$$

Since all eigenvalues are not integers for Toluene, we conclude that $\mathcal{G}$ is not $\mathcal{DL}$-integral. The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{&[26.1502]^1,\ [28.8272]^1,\ [30.3735]^1,\ [31.8487]^1,\ [34.8305]^1,\ [36.5582]^1,\\ &[38.3618]^1,\ [42.2155]^1,\ [43.0083]^1,\ [43.9083]^1,\ [46.1267]^1,\ [48]^2,\ [48.5445]^1,\\ &[89.2464]^1\}\end{aligned}$$

Given that $\text{trace}(\mathcal{DQ}(\mathcal{G})) = 636$ and $n = 15$, the average is $\frac{636}{15} = 42.4$, so the corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{15}|\gamma_i - 42.4| \approx 140.0686.$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{&[26.1502]^1,\ [28.8272]^1,\ [30.3735]^1,\ [31.8487]^1,\ [34.8305]^1,\\ &[36.5582]^1,\ [38.3618]^1,\ [42.2155]^1,\ [43.0083]^1,\ [43.9083]^1,\\ &[46.1267]^1,\ [48]^2,\ [48.5445]^1,\ [89.2464]^1\}.\end{aligned}$$

Since not all eigenvalues are integers for Toluene, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

4.15. Cyclohexane (C_6H_{12})-Skeleton Bond Line

A *cycle graph* C_6, where six carbon atoms are arranged in a ring, with each carbon bonded to two hydrogen atoms, is shown in Figure 8 The cyclic structure of cyclohexane can be represented as a cycle graph, and readers can study the molecular stability and symmetry using its spectral properties. The distance matrix and Laplacian matrix will give insights into the overall symmetry and distances between atoms in the ring structure.

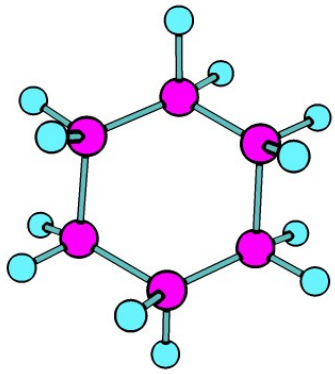

Figure 8. Cyclohexane (C_6H_{12}).

4.16. Spectral Properties of Cyclohexane (C_6H_{12})

Using chemical graph theory, we analyze its spectral matrices, related energies, and integrals. Let the vertex labeling be:

$$\begin{aligned} V(\mathcal{G}) =& \{v_1 = \mathrm{C}_1, v_2 = \mathrm{C}_2, v_3 = \mathrm{C}_3, v_4 = \mathrm{C}_4, v_5 = \mathrm{C}_5, v_6 = \mathrm{C}_6, v_7 = \mathrm{H}_1(\text{on } \mathrm{C}_1)\,, \\ & v_8 = \mathrm{H}_2(\text{on } \mathrm{C}_1),\ v_9 = \mathrm{H}_3(\text{on } \mathrm{C}_2)\, v_{10} = \mathrm{H}_4(\text{on } \mathrm{C}_2),\ v_{11} = \mathrm{H}_5(\text{on } \mathrm{C}_3), \\ & v_{12} = \mathrm{H}_6(\text{on } \mathrm{C}_3),\ v_{13} = \mathrm{H}_7(\text{on } \mathrm{C}_4),\ v_{14} = \mathrm{H}_8(\text{on } \mathrm{C}_4),\ v_{15} = \mathrm{H}_9(\text{on } \mathrm{C}_5), \\ & v_{16} = \mathrm{H}_5(\text{on } \mathrm{C}_5),\ v_{17} = \mathrm{H}_{11}(\text{on } \mathrm{C}_6),\ v_{18} = \mathrm{H}_{12}(\text{on } \mathrm{C}_6)\}. \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ for the molecular graph of Cyclohexane (C_6H_{12}) are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-13.4031]^2,\ [-4.5616]^1,\ [-2]^8,\ [-1.7726]^1,\ [-0.5969]^2,\ [-0.4384]^1, \\ &[-0]^2,\ [50.7726]^1\}. \end{aligned}$$

The corresponding distance energy is given by:

$$\begin{aligned} \mathcal{E}_{\mathcal{D}}(\mathcal{G}) = \sum_{i=1}^{10} |\alpha_i| &= 2|-13.4031| + |-4.5616| + 8|-2| + |-1.7726| + 2|-0.5969| \\ &+ |-0.4384| + 2|-0| + |50.7726| \approx 101.5452. \end{aligned}$$

The eigenvalues of the distance matrix $\mathcal{D}(\mathcal{G})$ are:

$$\begin{aligned} \mathcal{D}\text{-spec}(\mathcal{G}) = \{&[-13.4031]^2,\ [-4.5616]^1,\ [-2]^8,\ [-1.7726]^1, \\ &[-0.5969]^2,\ [-0.4384]^1,\ [-0]^2,\ [50.7726]^1\}. \end{aligned}$$

Since not all eigenvalues are integers for Cyclohexane, we conclude that $\mathcal{G}$ is not $\mathcal{D}$-integral. The diagonal transmission matrix is:

$$\mathcal{T}(\mathcal{G}) = \mathrm{diag}(39, 39, 39, 39, 39, 39, 55, 55, 55, 55, 55, 55, 55, 55, 55, 55, 55, 55)$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned} \mathcal{DL}\text{-spec}(\mathcal{G}) = \{&[-0]^1,\ [39]^1,\ [39]^1,\ [39.8953]^1,\ [41.6307]^2,\ [45]^1,\ [57]^8,\ [59.1047]^1, \\ &[66.3693]^2\}. \end{aligned}$$

Given that trace$(\mathcal{DL}(\mathcal{G})) = 894$, and $n = 18$, the average is $\frac{894}{18} \approx 49.6667$, so the distance Laplacian energy is given by:

$$\begin{aligned}\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) &= \sum_{i=1}^{18}\left|\beta_i - \frac{\text{trace}(\mathcal{DL}(\mathcal{G}))}{n}\right|,\\ &= \sum_{i=1}^{18}\left|\beta_i - \frac{894}{18}\right| = \sum_{i=1}^{18}|\beta_i - 49.6667| \approx 203.02.\end{aligned}$$

The eigenvalues of the distance Laplacian matrix $\mathcal{DL}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DL}\text{-spec}(\mathcal{G}) = \{&[-0]^1,\ [39]^1,\ [39]^1,\ [39.8953]^1,\ [41.6307]^2,\ [45]^1,\ [57]^8,\\ &[59.1047]^1,\ [66.3693]^2\},\end{aligned}$$

Since all eigenvalues are not integers for Cyclohexane, we conclude that $\mathcal{G}$ is not $\mathcal{DL}$-integral. The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{&[32.4502]^1,\ [32.4502]^1,\ [37.8479]^1,\ [39]^2,\ [39.8417]^1,\ [47.5498]^2,\\ &[51.1521]^1,\ [53]^8,\ [103.1583]^1\}.\end{aligned}$$

Given that trace$(DQ(\mathcal{G})) = 894$ and $n = 18$, the average is $\frac{636}{15} = 49.6667$, the corresponding $\mathcal{DQ}$-energy is given by:

$$\mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) = \sum_{i=1}^{18}|\gamma_i - 49.6667| \approx 163.2875.$$

The eigenvalues of the distance signless Laplacian matrix $\mathcal{DQ}(\mathcal{G})$ are:

$$\begin{aligned}\mathcal{DQ}\text{-spec}(\mathcal{G}) = \{&[32.4502]^1,\ [32.4502]^1,\ [37.8479]^1,\ [39]^2,\ [39.8417]^1,\\ &[47.5498]^2,\ [51.1521]^1,\ [53]^8,\ [103.1583]^1\}.\end{aligned}$$

Since not all eigenvalues are integers for Cyclohexane, we conclude that $\mathcal{G}$ is not $\mathcal{DQ}$-integral.

5. Comparative Analysis

A comparative analysis of spectral integrality across different distance-based matrices reveals that none of the selected chemical graphs exhibits fully integral spectra for all considered matrices. Nevertheless, the distance Laplacian spectrum displays integrality in certain cases (notably Methane and Formaldehyde), indicating that it tends to produce integral eigenvalues more often than the distance spectrum and the distance signless Laplacian spectrum. The basic graph parameters of the selected chemical structures, including the total number of vertices and edges, are summarized in Table 1.

Table 1. Basic graph parameters of selected chemical structures.

Chemical Graph	Chemical Formula	No. of Vertices	No. of Edges
Formaldehyde	CH_2O	4	3
Methane	CH_4	5	4
Methanol	CH_3OH	6	5
Ethylene	C_2H_4	6	5
Ethylene Glycol	$C_2H_6O_2$	10	9
Benzene	C_6H_6	12	12
Toluene	C_7H_8	15	15
Cyclohexane	C_6H_{12}	18	18

Correlation analysis of spectral energies across the selected molecular structures is presented in Table 2.

To investigate how spectral energies vary with molecular complexity, a comparative plot of the distance energy ($\mathcal{E}_{\mathcal{D}}$), distance Laplacian energy ($\mathcal{E}_{\mathcal{DL}}$), and distance signless Laplacian energy ($\mathcal{E}_{\mathcal{DQ}}$) for various chemical structures is provided. As shown in the figure, simpler molecules such as methane (CH_4) and formaldehyde (CH_2O) exhibit comparatively low spectral energy values across all three matrix types. In contrast, larger and more structurally complex molecules, such as benzene (C_6H_6) and toluene ($C_6H_5CH_3$), display significantly higher energy values, especially in the $\mathcal{E}_{\mathcal{DL}}$ and $\mathcal{E}_{\mathcal{DQ}}$ spectra.

It is observed that

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) > \mathcal{E}_{\mathcal{D}}(\mathcal{G}) \quad \text{and} \quad \mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) > \mathcal{E}_{\mathcal{D}}(\mathcal{G}).$$

Furthermore, according to Table 2, the following ordering consistently holds:

$$\mathcal{E}_{\mathcal{DL}}(\mathcal{G}) > \mathcal{E}_{\mathcal{DQ}}(\mathcal{G}) > \mathcal{E}_{\mathcal{D}}(\mathcal{G}).$$

Notably, the distance Laplacian energy ($\mathcal{E}_{\mathcal{DL}}$) increases more rapidly with growing molecular complexity than either the distance energy ($\mathcal{E}_{\mathcal{D}}$) or the distance signless Laplacian energy ($\mathcal{E}_{\mathcal{DQ}}$). This behavior suggests that $\mathcal{E}_{\mathcal{DL}}$ is particularly sensitive to structural branching and overall molecular connectivity, rendering it a more effective descriptor of topological complexity in molecular graphs. The graphical representations not only corroborate the numerical findings but also visually emphasize the capability of graph-theoretical spectral invariants to capture and quantify essential structural features of molecules.

Table 2. Spectral energy properties of some chemical structures.

Graph	$\mathcal{D}$-Energy	$\mathcal{DL}$-Energy	$\mathcal{DQ}$-Energy
Formaldehyde	9.2915	10.0	9.9282
Methane	13.2112	15.60	14.05
Methanol	19.3404	23.2445	20.9983
Ethylene	19.9999	24.5498	21.56
Ethylene Glycol	46.0447	67.3755	59.8605
Benzene	59.6228	95.0099	82.9291
Toluene	87.2467	160.3099	140.0686
Cyclohexane	101.5452	203.02	163.2875

$\mathcal{D}$-integral graphs are rare, primarily due to the non-integer eigenvalues in the distance matrix $\mathcal{D}(\mathcal{G})$. In our context, a molecule is said to be $\mathcal{D}$-, $\mathcal{DL}$-, and $\mathcal{DQ}$-integral if every eigenvalue of its distance Laplacian matrix is an integer; molecules like methane and formaldehyde satisfy this due to their symmetric, transmission-regular structures, whereas others do not. The spectral integrality of the computed structures are given in Table 3.

Figure 9 presents a 3D line chart generated in Excel to visually compare the spectral integrality properties ($\mathcal{D}$-, $\mathcal{DL}$-, and $\mathcal{DQ}$integral) of various chemical structures. Figure 10 presents a comparative analysis of energies across different graphs. The computed spectra, energies, and integrals offer valuable insights into the underlying chemical properties of the molecular structures.

Table 3. Spectral integrality of some chemical structures.

Graph	$\mathcal{D}$-Integral	$\mathcal{DL}$-Integral	$\mathcal{DQ}$-Integral
Formaldehyde	no	yes, $\{[0]^1, [4]^1, [7]^2\}$	no
Methane	no	yes, $\{[0]^1, [5]^1, [9]^3\}$	no
Methanol	no	no	no
Ethylene	no	no	no
Ethylene Glycol	no	no	no
Benzene	no	no	no
Toluene	no	no	no
Cyclohexane	no	no	no

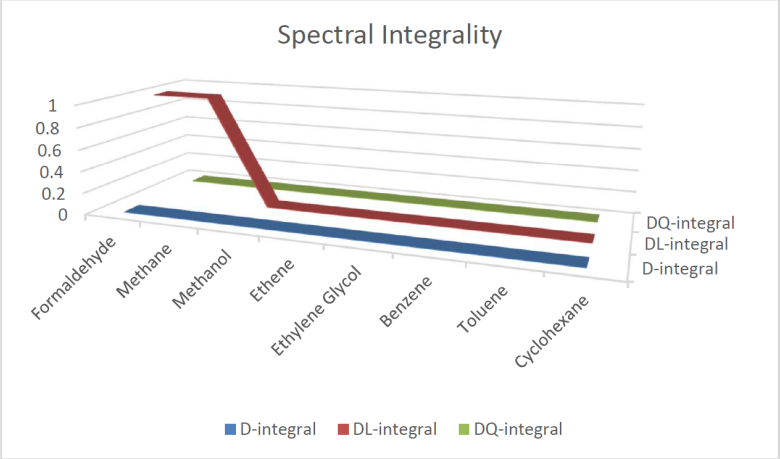

Figure 9. $\mathcal{D}/\mathcal{DL}/\mathcal{DQ}$-Integrality.

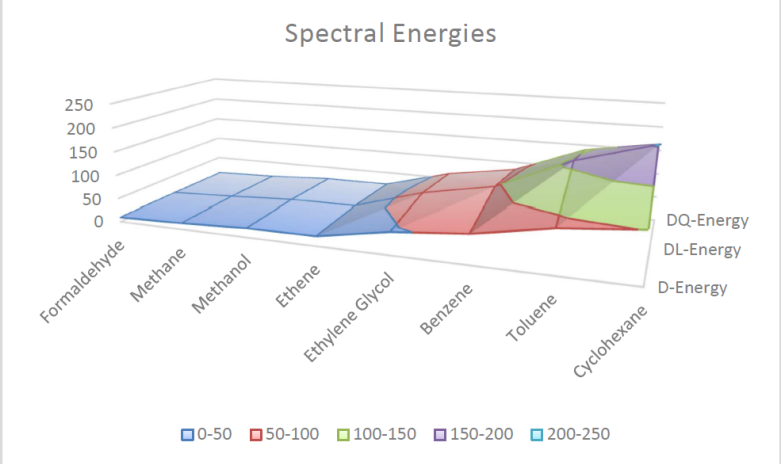

Figure 10. $\mathcal{D}/\mathcal{DL}/\mathcal{DQ}$-Energies.

6. Conclusions

This study highlights the effectiveness of distance-based spectral energies in analyzing molecular graphs corresponding to various chemical compounds, including Methane, Ethylene, Methanol, Formaldehyde, Benzene, Ethylene Glycol, Toluene, and Cyclohexane. By computing and comparing distance energy ($\mathcal{E}_{\mathcal{D}}$), distance Laplacian energy ($\mathcal{E}_{\mathcal{DL}}$), and distance signless Laplacian energy ($\mathcal{E}_{\mathcal{DQ}}$), we observed clear correlations between spectral metrics and molecular structural complexity. The results indicate that as molecular structures become larger and more topologically complex, their spectral energies, particularly $\mathcal{E}_{\mathcal{DL}}$ and $\mathcal{E}_{\mathcal{DQ}}$, increase substantially, highlighting the effectiveness of spectral graph theory

as a powerful analytical tool in mathematical chemistry. As per our observations, we conjecture that $\mathcal{E}_{\mathcal{DL}} > \mathcal{E}_{\mathcal{DQ}} > \mathcal{E}_{\mathcal{D}}$. The higher magnitude of distance Laplacian energy is attributed to the inclusion of vertex transmission terms, which capture global distance distributions and thus enhance sensitivity to molecular size, connectivity, and symmetry. The analysis of spectral integrality further reveals that most chemical structures exhibit non-integral spectra with respect to distance-based matrices, while a few, such as Methane and Formaldehyde, demonstrate integrality under the distance Laplacian matrix, emphasizing the role of molecular structure in determining spectral properties. Future research will focus on deriving analytical bounds and asymptotic formulas for distance-based energies over broader families of chemical graphs, as well as characterizing the structural conditions under which such inequalities persist or spectral integrality arises. Overall, this computational approach provides valuable insights into molecular stability and topology through a spectral perspective and opens avenues for deeper theoretical investigations.

Author Contributions: M.M.: Performed computations, prepared tables, and wrote the initial draft. S.A.: Defined the problem, created graphs, and prepared the final draft. A.A.L.: Verified calculations, reviewed the write-up, and approved the final version. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

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