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Article

Minimum Total Dominating Energy in Some Chemical Graphs

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Abstract: : A graph $\mathcal{G}$ = ($\curlyvee(\mathcal{G})$, $\mathcal{E}(\mathcal{G})$) is defined by an edge set $\mathcal{E}(\mathcal{G})$ and a vertex set $\curlyvee(\mathcal{G})$. When every vertex in a subset $\mathbb{S} \subseteq (\mathcal{G})$ is adjacent to at least one vertex in $\mathbb{S}$, the subset is referred to as a total dominating set (TDS). This means that every vertex must share an edge with at least one member of the set; no vertex is isolated or unrelated to the set $\mathbb{S}$. The smallest size of such a total dominating set is the total domination number (TDN), represented as $\gamma_t(\mathcal{G})$. It stands for the minimum number of vertices required to "cover" the graph in such a way that every other vertex is next to at least one of them. Additionally, the total dominating energy (TDE) of a graph, denoted $\mathcal{E}_{TD}(\mathcal{G})$, is calculated as the sum of the absolute values of all the Eigenvalues of the adjacency matrix of G. This energy concept provides insight into the structural properties and stability of a graph, and when applied to molecular graphs, it can help characterize chemical compounds in terms of graph-based descriptors.

This study calculates the minimal total dominant energy $\mathcal{E}_{TD}(\mathcal{G})$for the molecular graphs of a number of compounds, including sodium chloride, acetaminophen, chloroquine, sesame, and washing soda. In order to better understand the role of TDE in examining molecular stability and efficiency based on graph theoretical models; these compounds were chosen to investigate how their structural configurations affect their graph energies.
Keywords: Dominating-set (DS), Total Dominating-set, Total Dominating Number, Energy, Total Dominating-set Energy

1. INTRODUCTION

Domination theory in graphs was first studied mathematically in 1960. The idea of a graph's energy was first initiated by I. Gutman in 1978. The idea's beginnings can be traced back to C.F. De Jaenisch's investigation of the issue concluding the bare least number of queens needed to protect a $n \times n$ chessboard in such a way that each square is assaulted by a queen in 1862 [9].$\gamma_t(G)$ is the TDN of G, which is the minimal cardinality of a TDS of G. If a set S of vertices plotted in a graph $G(\curlyvee, E)$ is known as a TDS if all vertex v belongs to the $\curlyvee$ is adjacent to the element in$S$.The total electron energy of conjugated hydrocarbon molecules is a chemical property with strong ties to the graph invariant. The realm of chemistry is where the study of graph energy initially emerges. Chemists may use Huckel's type of method to estimate the energies of π-electron orbitales in the specific family of molecules called conjugated hydrocarbons. For a simple graph, Gutman was the first to establish the idea of "energy of graph." At first, it appeared that very few mathematicians were interested in this idea. However, graph energy has developed into an intriguing field of study for mathematicians throughout time, and a number of variants have been developed.[9]

In chemical graph theory, molecules have been shown as graphs, with an atom as vertices, chemical bonds as edges; under this model, the notion of dominance is of considerable importance. Parallel bonds stand in for double bonds. Chemical graph theory is an effective tool for comprehending how molecules behave, including their reactivity, stability, and physical characteristics. Additionally, it has uses in material science, other branches of chemistry and medication creation. The structure of the underlying linear change is shown by the eigenvalues and eigenvectors [3]. The energy of a graph is the absolute sum of its adjacency matrix's eigenvalues [4, 6]. Drugs like acetaminophen, chloroquine, sesame, washing soda and sodium chloride can be used in the mathematical aspects of graph energy can be referred in [7,11]. Further, studies are maximum degree energy [9], minimum dominating energy [10], Laplacian minimum dominating energy [10] and minimum covering distance energies [12]. In this study, the minimal TDE of $E_{TD}(G)$, in acetaminophen, chloroquine, sesame, washing soda and sodium chloride are computed.

Assume that G is a connected graph which contains p −vertices and also with q-edges. Consider $A = (a_{ij})$ represent the graph's adjacency matrix. Assume that a graph G has an adjacency matrix denoted by $\lambda_1,\ \lambda_2,\ \lambda_3, \dots \lambda_n$ has eigen values. A non-decreasing order is used to list the values. i.e., $\lambda_1, \geq \lambda_2, \geq \lambda_3, \geq \cdots \geq \lambda_n$. an eigenvalues of $A(G)$ are real numbers since $A(G)$ is a real and also it is symmetric. The energy $E(G)$ of a graph is defined as the sum of its eigenvalues in absolute terms, i.e., $E(G) = \sum_{i=1}^{n} |\lambda_i|$. [9]

1. **PRELIMINARIES**

Def:2.1 Dominating set

A DS for $G = (\Upsilon, E)$ is said to be subset D of Υ where all vertex not contain in Dit is adjacent to at least one of the members D. The term "domination number in G" (represented by the symbol$\gamma(G)$) refers to the least cardinality of a set of G that is DS[2][8].

Def:2.2 Total Dominating set

If every vertex $v \in \Upsilon$ is adjacent to an element of S, then the set S of vertices in D a graph $G(\Upsilon, E)$ is said to be a TDS. The TDN of G, represented by $\gamma_t(G)$, is the minimum cardinality of a TDS of G[1][9].

Def:2.3 Energy

The total of the absolute values of the eigenvalues of an adjacency matrix A, indicated as $E(\ G)$, is the energy of a connected graph $G = (\Upsilon, E)$ with the adjacency matrix called A. Specifically, $E(G) = \sum_{i=1}^{n} |\lambda_i|$ here λ_i is an eigenvalue in $A,\ i = 1,2,3, \dots n$[4][5].

Def: 2.4 The Minimum TDE

Consider G be a finite, connected graph with vertex Υ and edge E. If all of the vertex in a set, S in a graph G is next to a component of S, then S is a TDS. The TDN of G is the least cardinality over all minimal TDS of G. Let TDS stand for the smallest TDS of graph G.The least TDM of G is the square matrix ATD. $A_{TD}(G) = (a_{ij})$, equals(a_{ij}), where

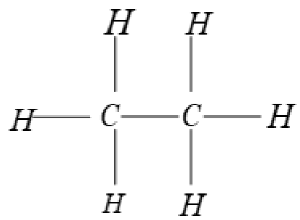
$$a_{ij} = \{ 1 \quad if \ \ v_i, v_j \ are\ adjacent \ 1 \quad if\ i = j, \quad v_i \in TDS \quad 0 \quad otherwise$$

The $f\ (G, \lambda\ )$ symbol stands for the characteristic polynomial of $A_{TD}(G) = (a_{ij})$, where $f\ (G, \lambda\ ) = det\ (\lambda I - A_{TD}(G))$. The minimal total dominating eigenvalues of the graph G are the eigenvalues of $A_{TD}(G)$. $A_{TD}(G)$ is symmetric and real, hence its eigenvalues are $\lambda_1, \lambda_2, \lambda_3 \dots \lambda_n$. in descending order $\lambda_1, \geq \lambda_2, \ \geq \lambda_3, \ \geq \cdots \geq \lambda_n$. $E_{TD}(G) = \sum_{i=1}^{n} |\lambda_i|$ is the formula for the total dominant energy of G.[10][12]

Example: Presume that $G = (\Upsilon, E)$ be a molecular graph of Ethane(C_2H_6), with $\Upsilon = \{ v_1,\ v_2,\ v_3,\ v_4, v_5, v_6,\ v_7,\ v_8\}$ is shown in Figures. The minimum TDS of Ethane is $\{v_3, v_6\}$ with minimum cardinality 2.

We use the following assumption for the diagrams

- Total domination set is considered with white vertices.



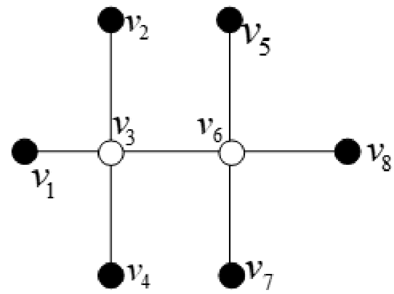


Figure: (a) Ethane's Chemical Structure (b) Molecular graph of Ethane

The minimum TD matrix,

$$A_{TD}\,(G)\ = (\quad)$$

The polynomial characteristic of G is

$$A_{TD}\,(G) = (\quad)$$

The characteristic equations are $\lambda^8 - 2\lambda^7 - 6\lambda^6 + 6\lambda^5 + 9\lambda^4 + 0\lambda^3 + 0\lambda^2 + 0\lambda = 0$

The Eigen values of G are 3.0000,-1.0000,-0.0000, -0.0000, 0.0000,0.0000, 1.7321, -1.7321.

∴ The minimum TDE, $E_{TD}(G) \approx 7.4642$

2. Analysis of Total Domination Energy in Chemical Graphs Structure:

This section discusses the calculation of the TDE for the molecular form graphs of specific compounds, including acetaminophen, chloroquine, sesame, washing soda and sodium chloride.

Observation 3.1: The TDE of acetaminophen is 16.788

Proof:

Let AC represent the acetaminophen molecular form graph, which has 13-vertices and 17- edges. Acetaminophen's chemical make-up and molecular map are exhibited in Figures 3.1(a) and 3.1(b), respectively.

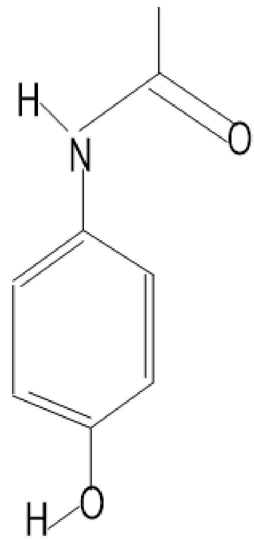
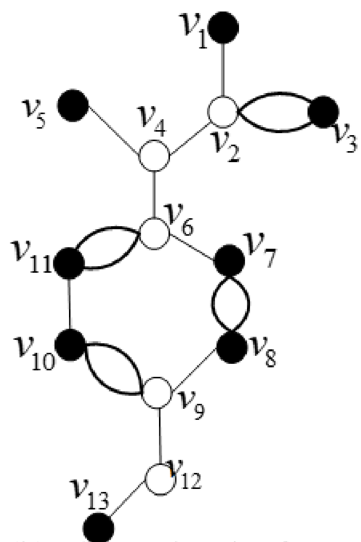


Figure 3.1: (a) Chemical form of Acetaminophen.



(b) The Molecular form of a Acetaminphen.

The least TDS of AC is $\{v_2, v_4, v_6, v_9, v_{12}\}$.

The TDS of acetaminophen has a minimum cardinality of five.

The minimum TD matrix, $A_{TD}(AC) = (\quad)$

The Characteristic polynomial of AC is

$$A_{TD}(AC) = (\quad)$$

The characteristic equation = $\lambda^{13} - 5\lambda^{12} - 3\lambda^{11} + 41\lambda^{10} - 11\lambda^9 - 124\lambda^8 + 43\lambda^7 + 176\lambda^6 - 38\lambda^5 - 119\lambda^4 + 2\lambda^3 + 31\lambda^2 + 6\lambda.$

Here we have the eigen values of AC, $\lambda_1 = 0.0000$, $\lambda_2 = 1.0000$, $\lambda_3 = -1.0000$, $\lambda_4 = -1.8522$, $\lambda_5 = -1.3303$, $\lambda_6 = -0.8847$, $\lambda_7 = -0.5819$, $\lambda_8 = -0.2449$, $\lambda_9 = 0.9209$, $\lambda_{10} = 1.3017$, $\lambda_{11} = 2.0388$, $\lambda_{12} = 2.6485$, $\lambda_{13} = 2.9841.$

∴The minimum TDE, $E_{TD}(AC) \approx 16.788$

Observation 3.2: The TDE of a chloroquine is 31.5711.

Proof:

Consider CH with 24-vertices, 30-edge chemical graph of chloroquine. Figures 3.2(a) and 3.2(b), respectively, display the molecular graph and chemical makeup of chloroquine.

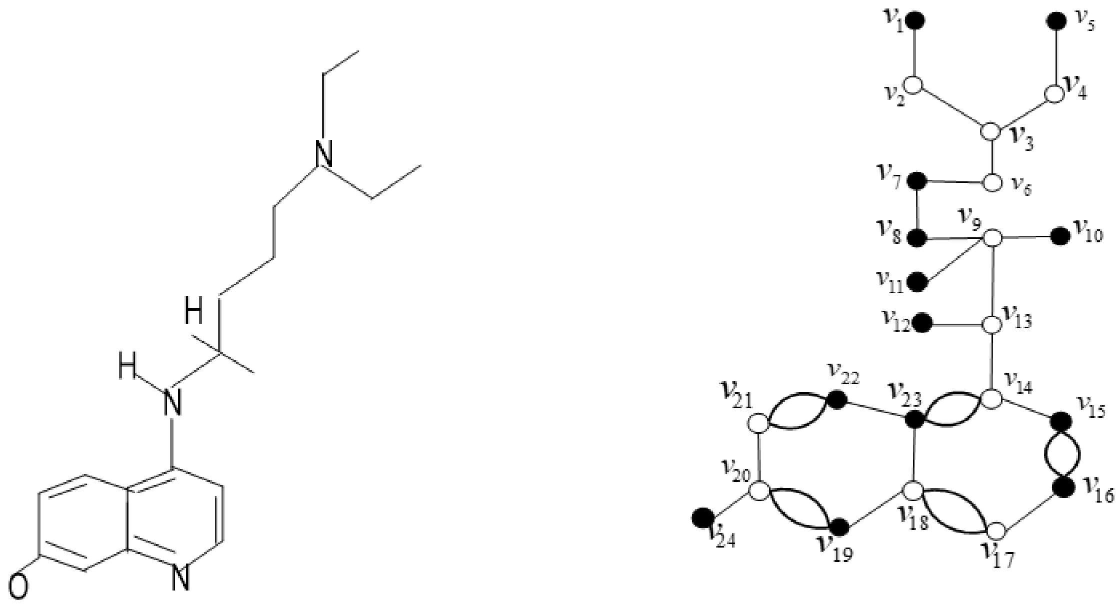


Figure 3.2: (a) Chloroquine's Chemical Structure (b) Chloroquine's Molecular Graph

The least TDS of CH is $\{v_2, v_3, v_4, v_6, v_9, v_{13}, v_{14}, v_{17}, v_{18}, v_{20,} v_{21}\}$.

The least cardinality of a TDS of chloroquine is 11.

The least TD matrix,

$$A_{TD}(CL) = \begin{pmatrix}
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&1&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&0&0&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&0&0\\
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0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0
\end{pmatrix}$$

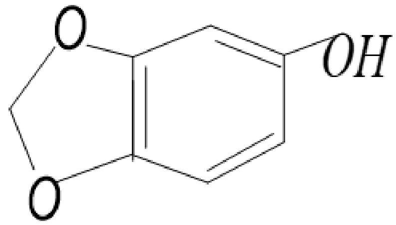
The characteristic equation is $\lambda^{24} - 11\lambda^{23} + 30\lambda^{22} + 81\lambda^{21} - 497\lambda^{20} + 115\lambda^{19} + 2849\lambda^{18} - 2960\lambda^{17} - 8491\lambda^{16} + 12685\lambda^{15} + 15112\lambda^{14} - 27344\lambda^{13} - 17655\lambda^{12} + 34026\lambda^{11} + 14854\lambda^{10} - 24668\lambda^{9} - 9264\lambda^{8} + 9591\lambda^{7} + 3679\lambda^{6} - 1543\lambda^{5} - 629\lambda^{4} + 30\lambda^{3} + 11\lambda^{2}$.

Here we have the eigen values λ_1= -1.9744, λ_2 = -1.7212, λ_3 = -1.3887, λ_4 = -1.2221, λ_5 = -1.0868, λ_6 = -0.9239, λ_7 = -0.6360, λ_8 = -0.6180, λ_9 = -0.5795, λ_{10} = -0.1354, λ_{11} = 0.0000, λ_{12} = 0.0000, λ_{13} = 0.1425, λ_{14} = 0.6066, λ_{15} = 1.0094, λ_{16} = 1.3362, λ_{17} = 1.4380, λ_{18} = 1.6180, λ_{19} = 1.7001, λ_{20} = 2.1052, λ_{21} = 2.4396, λ_{22} = 2.8396, λ_{23} = 2.9247, λ_{24} = 3.1252.

∴The minimum TDE of chloroquine, $E_{TD}(CH) \approx 31.5711$

Observation 3.3: The TDE of sesame is 14.0975

Consider SE to be the 11-vertices, 14-edge chemical graph of sesame ($C_7H_6O_3$). Figures 3.3(a) and 3.3(b), respectively, display the molecular graph and chemical makeup of sesame.



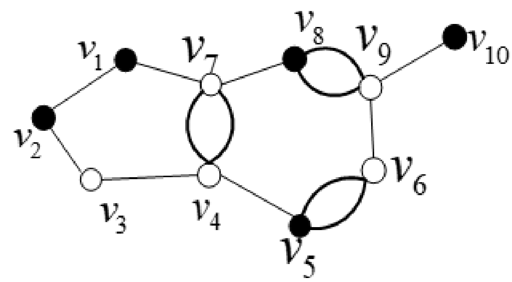


Figure 3.3: (a) Sesame'sChemical Structure. (b) Sesame'sMolecular Graph

The least TDS of SE is $\{v_3, v_4, v_6, v_7, v_9\}$.

The minimum cardinality of a TDS of sesame is 5.

The least TD matrix, $A_{TD}(SE) = (\quad)$

The Characteristic polynomial of SE is

$$A_{TD}(SE) = (\quad)$$

The characteristic equation is $\lambda^{10} - 5\lambda^9 - \lambda^8 + 32\lambda^7 - 16\lambda^6 - 70\lambda^5 + 38\lambda^4 + 61\lambda^3 - 21\lambda^2 - 18\lambda + 1$.

∴ *Here we have the eigen values* λ_1 = -1.6686, λ_2 = -1.3961, λ_3 = -0.8978, λ_4 = -0.5863,

λ_5 = 0.0528, λ_6 = 0.8632, λ_7 = 1.3560, λ_8 = 1.7433, λ_9 = 2.4662, λ_{10} = 3.0672.

∴ The minimum TDE of sesame, $E_{TD}\,(SE) \approx 14.0975$

Observation 3.4: The TDE of Sodium bicarbonate is 7.4134

Proof:

Consider SB to be the 6-vertices, 5-edge chemical graph of Sodium bicarbonate. Figures 3.4(a) and 3.4(b), respectively, display the molecular graph and chemical makeup of sodium bicarbonate.

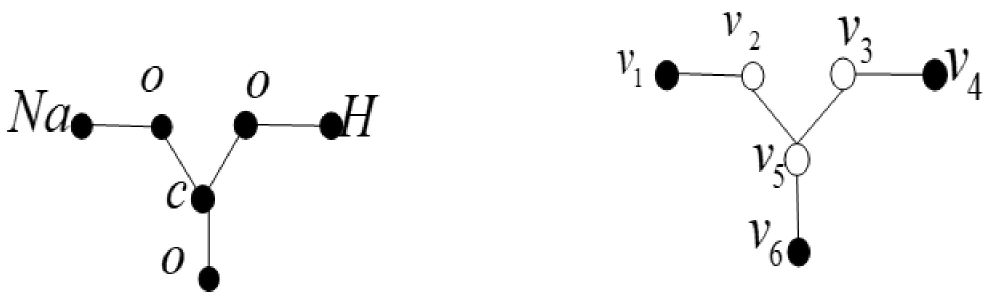


Figure 3.4: (a) Molecular structure of Sodium bicarbonate. (b) Chemical Graph of Sodium bicarbonate.

The minimum TDS of SB is $\{v_2, v_3, v_5\}$.

The minimum cardinality of TDS of Sodium bicarbonate is 3.

The minimum TD matrix,

$$A_{TD}(SB) = (\quad)$$

The Characteristic polynomial of SB is

$$A_{TD}(SB) = (\quad)$$

The characteristic equation is $\lambda^6 - 3\lambda^5 - 2\lambda^4 + 7\lambda^3 + 2\lambda^2 - 3\lambda - 1$.

Here we have the eigen values $\lambda_1 =$ -1.2283, λ_2= -0.6180, $\lambda_3 =$ -0.3604, $\lambda_4 =$ 0.8141, $\lambda_5 =$1.6180, $\lambda_6 =$2.7746.

∴ The minimum TDE of sodium bicarbonate, $E_{TD}(SB) \approx 7.4134$

Observation 3.5: The TDE of Sodium chloride is 44.5797

Consider SC to be the 27-vertices, 36-edge chemical graph of Sodium chloride. Figures 3.5(A) and 3.5(B), respectively, display the molecular graph and chemical makeup of sodium chloride.

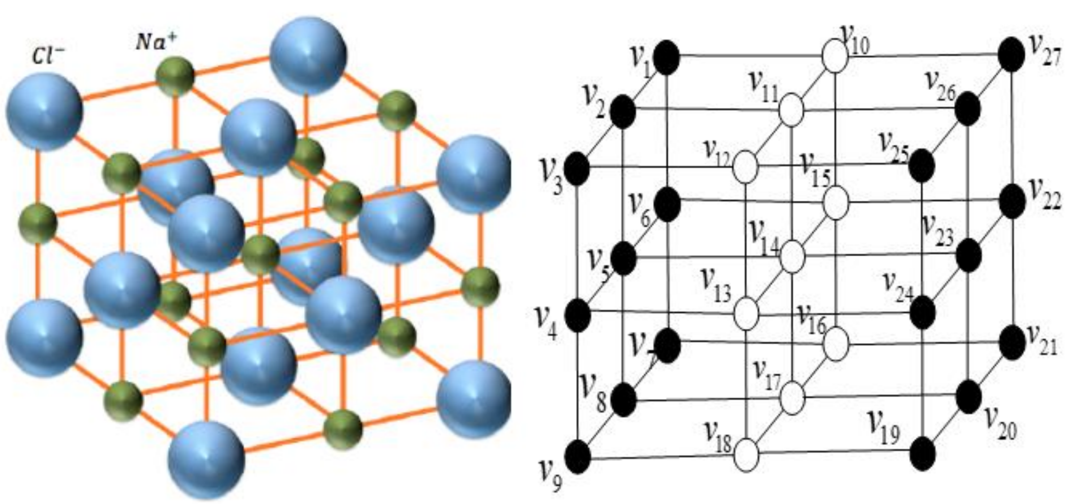


Figure 3.5: (a) Molecular form of sodium chloride. (b) Sodium chloride's chemical form in graph.

The least TDS of SC is $\{v_{10}, v_{11}, v_{12}, v_{13}, v_{14}, v_{15}, v_{16}, v_{17}, v_{18}\}$.

The minimum cardinality of TDS of sodium chloride = 9.

The minimum TD matrix,

$$A_{TD}(sc) = (\quad)$$

The characteristic equation is $\lambda^{27} - 9\lambda^{26} - 18\lambda^{25} + 360\lambda^{24} - 306\lambda^{23} - 5574\lambda^{22} + 10716\lambda^{21} + 43152\lambda^{20} - 117207\lambda^{19} - 175721\lambda^{18} + 663606\lambda^{17} + 336408\lambda^{16} - 2180088\lambda^{15} - 39048\lambda^{14} + 4333584\lambda^{13} - 1089664\lambda^{12} - 5218224\lambda^{11} + 2166768\lambda^{10} + 3631328\lambda^{9} - 1964928\lambda^{8} - 1257984\lambda^{7} + 897280\lambda^{6} + 109056\lambda^{5} - 165888\lambda^{4} + 28672\lambda^{3}$.

Here we have the eigen values λ_1= 4.7863, $\lambda_2 =$-3.7910, $\lambda_3 =$3.4142, $\lambda_4 =$3.2045, $\lambda_5 =$ -2.8284, $\lambda_6 =$2.8284, $\lambda_7 =$ -2.4492, $\lambda_8 =$ -2.4142, $\lambda_9 =$2.0000, $\lambda_{10} =$2.0000, $\lambda_{11} =$1.8515, $\lambda_{12} =$1.6230, $\lambda_{13} =$ -1.4142, $\lambda_{14} =$-1.4142, $\lambda_{15} =$1.4142, $\lambda_{16} =$1.4142, $\lambda_{17} =$-1.1917, $\lambda_{18} =$-1.0000, $\lambda_{19} =$-1.0000, $\lambda_{20} = -0.7870$, $\lambda_{21} =$0.5857, $\lambda_{22} =$0.5569, $\lambda_{23} =$0.4142, $\lambda_{24} =$0.1967, $\lambda_{25} = 0.0000$, $\lambda_{26} = 0.0000$, $\lambda_{27} = 0.0000$.

∴ The minimum TDE of sodium chloride, $E_{TD}\ (SC) \approx 44.5797$

3. Conclusion:

This study investigates the idea of least total domination energy (least TDE) in relation to molecular graphs of a number of different chemical substances, such as washing soda, sodium chloride, acetaminophen, chloroquine, and sesame. Atoms are shown as vertices in a molecular graph, while bonds are shown as edges. The least TDE, which functions as a structural descriptor for the compound, is obtained from the fewest eigenvalues of the graph's total domination matrix.
Understanding the chemical and topological characteristics of molecular structures can be gained by computing the least TDE. Understanding molecule stability and reactivity is one area in which it is especially helpful. To illustrate the relevance and usefulness of this metric, the least TDE values are calculated for both real chemical compounds and often researched graph topologies.

Since TDE has the ability to analyse properties in more general mathematical and theoretical graph models, it can be used in fields other than chemistry. Researchers can better understand molecules mathematically by interpreting chemical structures using this energy-based viewpoint. This insight could help advance cheminformatics, drug design, and computational chemistry. Overall, this study advances the creation of energy-based molecular descriptors as well as chemical graph theory.

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