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# Analyzing the Reducing Strength of Oxalic Acid and Sodium Thiosulfate through Graph Theory

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***Abstract*— This research evaluates the plummeting controls of sodium thiosulfate ($Na_2S_2O_3$) and oxalic acid ($C_2H_2O_4$) using graph theory. The molecular structure of each molecule was modelled using Laplacian matrices. Oxalic acid was found to have lower index values using topological index analysis, but sodium thiosulfate displayed greater values. In addition, eigenvalue analysis shows that sodium thiosulfate has a larger spectral radius than oxalic acid, suggesting a stronger electron transfer potential. These outcomes are dependable with experimental indication, proving the helpfulness of graph theory in chemical studies and corroborative that sodium thiosulfate has a higher reducing power.**

***Keywords*— Topological indices; Laplacian Matrix; Sodium thiosulfate; Oxalic acid.**
**2020 Mathematics Subject Classification: 05C50; 15A18; 05C22.**

## I. INTRODUCTION

A strong foundation for examining a material's atomic and molecular structure and chemical characteristics is given by graph theory. Researchers can use mathematical models to study further regarding different material qualities by portraying atoms as vertices and bonds as edges in a graph. The stability, connectedness and reactivity of oxalic acid and sodium thiosulfate are examined via the lens of graph theory[1,2].

A fuzzy graph $G = (V, \mu, \rho)$ is a nonempty set $V$ together with a pair of functions $\mu: V \to [0, 1]$ and $\mu: V \times V \to [0, 1]$ such that for all $x, y$ in $V$, $\rho(x, y) \leq \mu(x) \wedge \mu(y)$. We call $\mu$ the *fuzzy vertex set* of $G$ and $\rho$ the *fuzzy edge set* of $G$, respectively. Note that $\rho$ is a fuzzy relation on $\mu$ [3].

The vertex set of the fuzzy graph in the chemical graph is the atoms and the bond represents the edge set.

The adjacency matrix N ($H$) of a graph is an n×n matrix where the entry is $\rho(uv)$ if two vertices are adjacent, and 0 otherwise. The diagonal matrix D ($H$) contains $\mu(v)$ on its diagonal where $v \in V$ and zeros elsewhere [4].

The Kirchhoff matrix, or Laplacian matrix B ($H$), is defined as

B($H$) =D($H$) −N ($H$). This matrix is symmetric and its eigenvalues, which are non-negative due to Gershgorin's theorem, provide important information about the graph's structure [5,6].

Reactivity and stability not only depend on the molecular crisp graph structure but also on atomic energy, bond energy, etc. for chemical compounds Oxalic Acid and Sodium Thiosulfate, we have constructed a fuzzy graph using atomic energy, bond energy. The vertex set of the fuzzy graph is the oxygen, carbon and hydrogen atoms, and the oxygen-carbon bond, hydrogen-oxygen bond and carbon-carbon bond represents the edge set. Similarly, in Sodium Thiosulfate there exists oxygen- sulfur bond and sulfur-sulfur bond represents the edge set, vertex set is sulfur and Oxygen atoms and we have vertex and edge membership values as:

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$$\mu(v) = \frac{Atomic\ energy\ of\ a\ vertex\ v}{Maximum\ atomic\ energy\ among\ all\ vertices}$$

$$\rho(uv) = \frac{Bond\ energy\ of\ the\ edge\ uv}{Maximum\ of\ atomic\ energy\ of\ u, v}$$

Clearly, $\mu(v) \in [0, 1], \forall\ v \in V$. Also, bond energy of the edge $uv$ is always less than atomic energy of end vertices, hence, $\rho(uv) \in [0, 1], \forall\ uv \in E$ and $\rho(uv) \leq \min\{\mu(u), \mu(v)\}, \forall\ uv \in E$. As the triplet $(V, \mu, \rho)$ satisfies all the criteria of a fuzzy graph, $(V, \mu, \rho)$ forms a fuzzy graph. Where V is the set of vertices, Observe that sulfur has an atomic energy of 999.6 kJ/mol while oxygen has an atomic energy of 1313.94 kJ/mol. , atomic energy of carbon is 1086.5kj/mol and the bond energy of O-S is 300 kJ/mol in double bond and single bond, O-C single bond is 350kj/mol, O-C double bond is 740kj/mol, C-C single bond is 348kj/mol and O-H single bond is 460kj/mol Using the above two formulae, we get $\mu(O) = 1.00$ , $\mu(S) = 0.7608$ , $\mu(H) = 0.99$, $\mu(C) = 0.826$, $\rho(O - S) = 0.23$, $\rho(O - H) = 0.35$, $\rho(C - C) = 0.32$, $\rho(O = C) = 0.563$, $\rho(O - C) = 0.27$.

The Laplacian matrix of $C_2H_2O_4$ and $Na_2S_2O_3$ are as follows:

$$\begin{pmatrix} 0.99 & 0.35 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.35 & 1.0 & 0.27 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.27 & 0.826 & 0.563 & 0.0 & 0.32 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.563 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.563 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.32 & 0.0 & 0.563 & 0.826 & 0.27 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.27 & 1.0 & 0.35 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.35 & 0.99 \end{pmatrix}$$

$$\begin{pmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.23 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.23 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.23 \\ 0.0 & 0.0 & 0.0 & 0.7608 & 0.2 \\ 0.23 & 0.23 & 0.23 & 0.2 & 0.7608 \end{pmatrix}$$

The eigenvalues of above matrices are:

TABLE I

| $C_2H_2O_4$ | $Na_2S_2O_3$ |
|---|---|
| 0.07245943265895932, | 0.3916055230979849, |
| 0.41241409222650977, | 1.3231058962509827, |
| 0.6749262449638743, | 1.0000000000000004, |
| 0.6990971037813589, | 0.8068885806510312, |
| 1.7190844286841118, | 1.0 |
| 1.4807445791609803, | |
| 1.2678697432161874, | |
| 1.305404375308018 | |

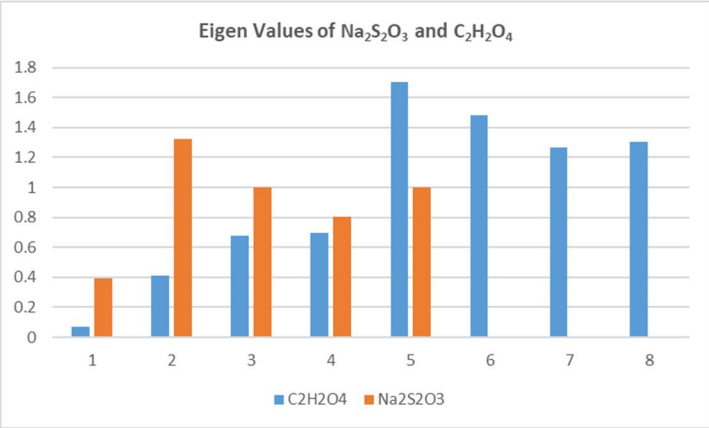


Figure 1

Oxalic acid is a stronger reducing agent than Sodium thiosulfate because it donates electrons more readily and can reduce a broader range of oxidizing agents.
Significance of Laplacian Matrix in Material Science: The Laplacian matrix's maximum eigenvalue $\eta_1$ is particularly significant in the study of chemical graphs, as it reflects key aspects of molecular structure, connectivity, and stability [7,8]. For the Laplacian matrix can offer insights into the anisotropic properties and connectivity within the lattice. The eigenvalues derived from this matrix can indicate the extent of connectivity and potential effects on properties such as electrical conductivity [2, 20]

*B. Characteristic Polynomial of the Laplacian Matrix*

The coefficients of the characteristic polynomial of the Laplacian matrix of the chemical graph of $C_2H_2O_4$ and $Na_2S_2O_3$ carry crucial information about the structure's connectedness, stability, and possible reactivity [9]. These coefficients can be used to forecast potential behaviors of $C_2H_2O_4$ and $Na_2S_2O_3$ in different chemical environments, identify potential regions of chemical reactivity, and get additional knowledge about the material's overall stability[10]. This approach provides a mathematical basis for relating the structural features of $C_2H_2O_4$ and $Na_2S_2O_3$ to their chemical properties.
The determinantal polynomial P($\eta$) for the Kirchoff matrix $L$ of a graph is typically expressed as: $P(\eta) = \eta^p + a_{p-1}\eta^{p-1} + a_{p-2}\eta^{p-2} + \cdots + a_1\eta + a_0$ where p is the size of the Kirchoff matrix (i.e., the number of vertices in the graph), and $a_i$ are the coefficients. From the Coefficients of Characteristic polynomial encodes crucial information about the graph's connectivity and stability. The coefficients of this polynomial reflect the structural robustness and potential reactivity of the material. For $C_2H_2O_4$ and $Na_2S_2O_3$ analysing these coefficients helps in understanding the material's stability, predicting reactive sites, and correlating these findings with its chemical properties[11].
The characteristic polynomials of $C_2H_2O_4$ and $Na_2S_2O_3$ are follows:
P($x$) =
$x^8-7.632x^7+24.334197999999997x^6-41.973574852x^5+42.329102762721x^4-25.104333005741978x^3+8.292605928005608x^2-1.3038956594051587x+0.059404494558356724$.
Q(y) =
$y^5-4.5216y^4+7.944916640000001y^3-6.743110960000002y^2+2.7378720000000025y-0.41807768000000056$

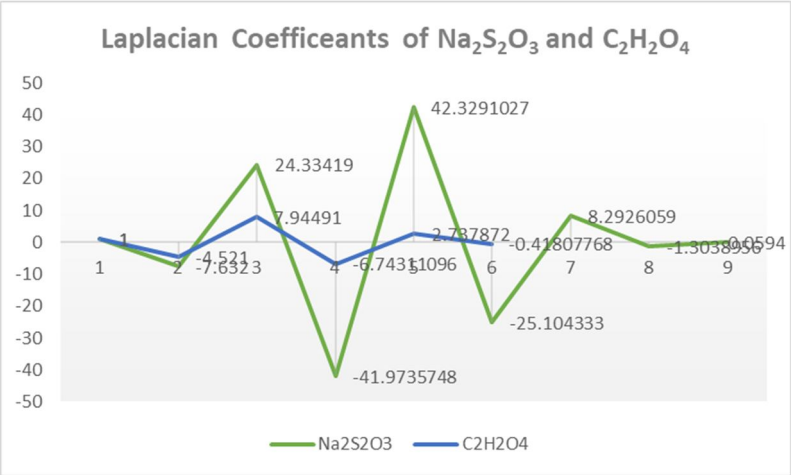


Fig.10 coefficients of characteristic polynomial

A chemical graph's characteristic polynomial's highest and lowest coefficients gives significant acumens about the structural elements of the substance. Although the lowest coefficient may indicate weak substructures, ability locations of unsteadiness, or fields of excessive reactivity, the highest coefficient typically indicates structural toughness, steadiness, and robust connection within the material[12]. By investigative these coefficients of the determinantal polynomial of the chemical graphs of $C_2H_2O_4$ and $Na_2S_2O_3$, one can progress understand their physical and chemical activities and see how steady, reactive, and other material attributes they are.
The least coefficient may point to fewer stable substructures or low points in the material. If a term with a lower power of $\eta$ is related with the smallest coefficient, it may be link up to subgraphs that are smaller and less bonded. These can be indicatory of undercoordinated atoms, fragile bonds, or defects, which can indicate to structural collapse or chemical reactions.

A very low (or negative) minimum coefficient might highlight a structural feature that contributes to higher reactivity. In $C_2H_2O_4$ and $Na_2S_2O_3$ a small coefficient might be related to a subgraph that corresponds to a reactive surface site or a defect in the crystal structure where chemical reactions are more likely to occur[13].

## II. Topological Indices

Topological Indices as Descriptors of Chemical Properties: Topological indices such as the First and Second Zagreb index offer additional insights into the material's properties. [14,23].

### *A. Topological Indices of $C_2H_2O_4$ and $Na_2S_2O_3$ chemical graph*

Topological indices are numerical values that are extracted from the structure of a chemical graph and assist as significant methods to know the properties of chemical compounds, with their stability, reactivity, and other physical and chemical characteristics[15-17,23].
Topological indices are broadly worked to foretell and represent the properties of chemical compounds. They are remarkably worthy, because they can compare with a broad range of properties, involving heating points, stability, reactivity, and biological movement, without expecting comprehensive quantum mechanical calculations[28].
Certain crucial indices and their values concerning $C_2H_2O_4$ and $Na_2S_2O_3$ are follows:

### *B. First Zagreb Index($M_1(H)$) [18]*

The sum of the squares of the degrees of each vertex in a graph is its first Zagreb index.
The first Zagreb index is defined as: $M_1(H) = \sum_{v \in V} d^2(v)$.

### *C. Second Zagreb Index($M_2(H)$)[19]*

The second Zagreb index of a graph is the summation of the product of degree of every pair of vertices which are adjacent in the graph.
The second Zagreb index is defined as: $M_2(H) = \sum_{u,v \in E} d(u)d(v)$.

### *D. F-Index (F (H)) [20]*

A graph's F-Index is calculated by adding the cube of each vertex's degree together.
The F- index is defined as: $\mathbf{F}(H) = \sum_{v \in V} d^3(v)$.

### *E. First Zagreb Index for the Fuzzy graph [21]:*

The first Zagreb index of a fuzzy graph (V, $\mu$, $\rho$) is the summation of the square of the degree of every vertex along with value of the atom in the graph.
The first Zagreb index is defined as: $M_1(H) = \sum_{v \in V} \mu(v)\, d^2(v)$.

### *F. Second Zagreb Index for the Fuzzy graph [22]*

The second Zagreb index of a fuzzy graph (V, $\mu$, $\rho$) is the summation of the product of degree of every pair of vertices along with their values of the atoms in the pair which are adjacent in the graph.
The second Zagreb index is defined as: $M_2(H) = \sum_{u,v \in E} \mu(u)\ d(u)\, d(v)\ \mu(v)$ .
The First Zagreb index and Second Zagreb index presents information about the complete connectivity and efficiency of the structure[26]. A lower value of above indices indicates a more compact structure, which might correlate with higher reactivity [20,24,25].
The different topological index of values are as follows:

TABLE II

| Topological Indices | $C_2H_2O_4$ | $Na_2S_2O_3$ |
|---|---|---|
| First Zagreb Index | 44.44 | 36.432 |
| Second Zagreb Index | 56.824 | 27.388 |

## IV. Conclusion

We compared the reducing strengths of oxalic acid ($C_2H_2O_4$) and sodium thiosulfate ($Na_2S_2O_3$) using mathematical and graph-theoretical tools, including eigenvalues of the Laplacian matrix, coefficients of the characteristic polynomial, and the First and Second Zagreb Indices. The analysis shows that oxalic acid demonstrates a higher reducing strength compared to sodium thiosulfate.

The First and Second Zagreb Indices of oxalic acid reveal greater molecular irregularity, which correlates with its higher reactivity and greater tendency to donate electrons in redox reactions. Additionally, the eigenvalues of the Laplacian matrix for oxalic acid suggest a more dynamic electronic structure, further supporting its enhanced reducing ability. In contrast, sodium thiosulfate, with higher Zagreb Indices and characteristic polynomial coefficients, displays a more stable and less reactive molecular configuration. From the above all parameters we provided the proof Mathematically that Oxalic acid is a stronger reducing agent than Sodium thiosulfate

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