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Research Article

Three-Dimensional Structural Modelling and Characterization of Sodalite Material Network concerning the Irregularity Topological Indices

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Topological characterization of 3D molecular structures is an emerging study area in theoretical and computational chemistry. These structural descriptors are used in a variety of domains, including chemical graph theory, drug delivery, and nanomaterial characterization. Quantitative structural descriptors can be used to characterize the chemical and physical properties of a given compound. Topological indices of molecular graphs are numerical quantities that allow us to collect information about the chemical structure and reveal its hidden qualities without performing experiments. Due to the low cost of implementation, zeolite networks are considered popular chemical networks. Zeolites are widely used networks with applications in chemistry, medicine, and commercial production owing to their excellent chemical features. The sodalite network is composed of a very unique type of zeolite framework called sodalite. It is a three-dimensional network of interconnected cages and tunnels that provide an ideal environment for a wide range of chemical and physical processes. This paper deals with the sodalite material network's degree-based and reverse degree-based irregularity indices. These indices provide a quantitative measure of the irregular behaviour of the sodalite material network. It can be used to identify areas of the network where irregular behaviour is occurring and to compare different networks to determine which is more irregular. Additionally, these indices can be used to monitor changes in irregularity over time, allowing us to measure the impact of any interventions that are implemented.

1. Introduction

Macromolecular strainers, also known as natural zeolites, have been investigated and studied thoroughly [1–3]. Zeolite networks are currently identical attractive chemical networks because of their low deployment costs. Presently, there are about 248 categories of zeolites and they can be recognized through their silicone aluminium (Si/Al) proportion existing in the atomic construction of zeolites which includes of building blocks of numerous complications showing channels and coops [4]. The sodalite network is one of the most extensively researched forms of zeolite networks. It contributes significantly to the elimination of greenhouse gases. Zeolite's unique molecular comprehension distinguishes it as significant and relevant. Natural zeolites are beneficial in bulk mineral applications due to their lower cost [5]. Zeolites are classified into different groups based on their size and complexity. The most extensively researched compounds among the various zeolite structures are synthetic compounds and minerals with crystal structures resembling those of sodalite [5]. Various biochemical properties of sodalite and zeolite form constructions in terms of molecular descriptors are investigated in [6–8].

The sodalites with the best thermodynamic stability are recognized as one of the best structures among all zeolites. Due to their crystallographic backgrounds, the sodalites are also significant. The fundamental topology of each cage of sodalites is represented by the six- and four-membered rings. These rings are also shared by two of the parallel cages. In sodalite, cavities are created using a custom-made mixture to trap molecules. Zeolites can be used to remove water and greenhouse gases as well. Some other studies on zeolites, sodalite, and their practical applications are discussed in [9].

The QSPR and QSAR models are effective tools for predicting the properties and activities of materials by showing the underlying topological aspects of the molecular structure. These practical structural information representations have applications in coding, database retrieval, physicochemical property prediction, and material and molecular biological activity prediction. One of the most significant components of QSPR/QSAR modelling is the use of topological indices, which are structural descriptors with the potential to predict features. Because the activity of molecules is dependent on their 3D structures and the relative ease with which these indices can be used in computing molecular properties when compared to numerically intensive quantum chemical computations, topological indices have emerged as important descriptors in the field of computational and theoretical chemistry [10–14].

A graph is called a regular graph if all of its vertices have the same degree. If the topological index associated with a graph is larger than or equal to zero, it is referred to as an "irregularity index," and if the graph is regular, the topological index will be zero. The main challenge in obtaining the irregularity topological index is the computational complexity associated with the calculation. This complexity arises from the need to consider all possible paths in a graph in order to determine its topological indices. Furthermore, the calculation of these indices is often computationally expensive due to the large number of nodes and edges that need to be considered. Additionally, the complexity of calculating these indices increases exponentially with the size of the graph. Finally, the calculation of the irregularity topological indices requires the use of sophisticated algorithms, which can be difficult to implement. The majority of irregularity indicators are degree-based topological indices that are utilized in quantitative activity relationship modelling [15]. In [16], Gutman introduced some new topological indices. Zaman and Ali [17] obtained the maximum connectivity index of a Halin graph. The Kirchhoff index and Laplacian graph vitality is presented by Zaman in [18–21]. Manzoor et al. in [22] and Ullah et al. in [23] obtained the entropy measures of molecular graphs using topological indices and also established the entropy measure of phthalocyanine and porphyrin dendrimers, respectively. The hyper–Wiener index for fuzzy graph and its application in the share market is accomplished in [24]. Further development of the F-index for fuzzy graph and its application in Indian railway crime are discussed in [25]. In [26], Zaman et al. determined the structural analysis and topological characterization of sudoku nanosheets. Ullah et al. computed the network-based modelling of fuchsine acid

dye's molecular topology in relation to various irregular molecular descriptors in [27]. The authors of [28] obtained a fresh look at the modelling and topological characterization of H-Naphtalenic nanosheets with applications. In [29], Zaman et al. introduced the maximum H-index of bipartite network with some parameters. In [30], Islam and Pal obtained the second Zagreb index for fuzzy graphs and its application in mathematical chemistry. The first Zagreb index on a fuzzy graph and its application are discussed in [31].

2. Preliminaries

Topological indices, also known as molecular descriptors, are mathematical formulas under molecular characteristics that can be used in the analysis of physical and chemical properties and are then used by medical researchers for drug development as it is a low-cost and quick-processing computational tool. Topological indices play a significant role in mathematical chemistry, more specifically in QSAR and QSPR analysis. There are numerous types of topological indices at present, including distance-based, degree-based, and eccentricity-based topological indices, which are widely used for chemical structure analysis. The following notations and definitions are important for our study. Let H be a graph with an edge set E and vertex set V. $|E|$ denotes size of a graph, and $|V|$ represents the total number of nodes or atoms. The irregularity index is a more efficient technique to express irregularity. Recently, a new approach of studying irregularity indices has been developed [32, 33]. The 1st irregularity index was introduced by Bell in 1992 [34]. Most of these indices used the concept of imbalance of an edge defined as $\text{imball}_{\mu v} = \left| d_\mu - d_v \right|$.

Recently, the authors computed irregularity indices for a family of nanotubes in [35]. The irregularity indices of some dendrimer structures are studied by Gao et al. in [36] and molecular structures in [37]. Hussain et al. computed these irregularity measures for some classes of benzenoid systems in [38]. Motivated by these works, we have investigated the degree-based and reverse degree-based irregularity indices for sodalite material networks.

The Albertson index, AL, was defined by Alberston and is defined as follows [39]:

$$AL(\mathbb{H}) = \sum_{\mu v \in E(\mathbb{H})} \left| d_\mu - d_v \right|. \tag{1}$$

In this index, the imbalance of edges is computed. The irregularity index IRL and IRLU are introduced by Kovačević and Gasparov, given as follows [40]:

$$IRL(\mathbb{H}) = \sum_{\mu v \in E(\mathbb{H})} \left| \ln d_\mu - \ln d_v \right|, \text{ and}$$

$$IRLU(\mathbb{H}) = \sum_{\mu v \in E(\mathbb{H})} \frac{\left| d_\mu - d_v \right|}{\min \left(d_\mu, d_v \right)}. \tag{2}$$

Recently, Abdoo and Dimitrov introduced the new term "total irregularity measure of a graph G," which is given as follows [41]:

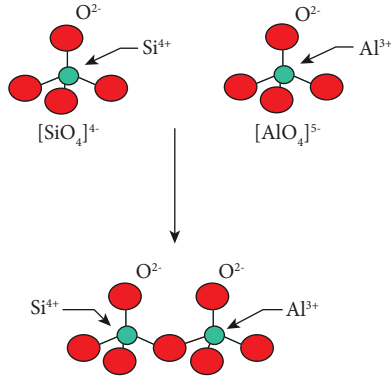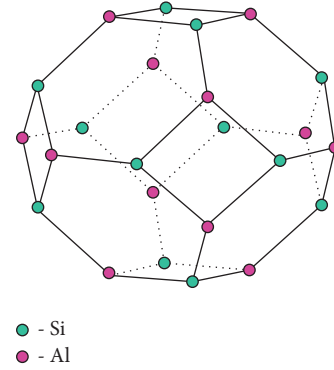FIGURE 1: Chemical graph of zeolites.

$$\mathrm{IRR}_t\left(\mathbb{H}\right) = \frac{1}{2} \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \left|d_\mu - d_\mathsf{v}\right|. \tag{3}$$

Recently, Gutman and Das introduced the IRF irregularity index of the graph, which is given as follows [42]:

$$\mathrm{IRF}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \left(d_\mu - d_\mathsf{v}\right)^2. \tag{4}$$

The Randic index itself is directly related to an irregularity measure, which is described as follows [15]:

$$\mathrm{IRA}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \left(d_\mu^{-1/2} - d_\mathsf{v}^{-1/2}\right)^2. \tag{5}$$

The detailed tracing of more irregularity indices of a similar nature is accessible [43]. These indices are given by

$$\mathrm{IRDIF}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \left|\frac{d_\mu}{d_\mathsf{v}} - \frac{d_\mathsf{v}}{d_\mu}\right|,$$

$$\mathrm{IRLF}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \frac{\left|d_\mu - d_\mathsf{v}\right|}{\sqrt{d_\mu d_\mathsf{v}}},$$

$$\mathrm{IRLA}\left(\mathbb{H}\right) = 2 \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \frac{\left|d_\mu - d_\mathsf{v}\right|}{\left(d_\mu + d_\mathsf{v}\right)}, \tag{6}$$

$$\mathrm{IRD1}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \ln\left\{1 + \left|d_\mu - d_\mathsf{v}\right|\right\},$$

$$\mathrm{IRGA}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \ln\frac{\left(d_\mu + d_\mathsf{v}\right)}{2\sqrt{d_\mu d_\mathsf{v}}},$$

$$\mathrm{IRB}\left(\mathbb{H}\right) = \sum_{\mu\mathsf{v}\in E(\mathbb{H})} \left(\sqrt{d_\mu} - \sqrt{d_\mathsf{v}}\right)^2.$$

3. Structure of Sodalite Materials

The chemical graph of zeolites is given in Figure 1. Commonly referred to as a "cage," the building block (or "unit

FIGURE 2: Unit cell of zeolite (β-cage).

cell") of sodalite structures is a truncated octahedron with 24 vertices and 36 edges and 6 squares and 8 hexagons joined by sharing a common edge as illustrated in Figure 2. The structurally interconnected arrangement of β − cages in the ḷ×ṃ mesh results in a single layer of sodalite materials, as shown in Figure 3, and this layer can be easily extended to many layers by arranging in ḷ×ṃ×ṇ mesh, denoted by SOD (ḷ,ṃ,ṇ), where p, q, r are parameters to show the copies of structure vertically (length), inside the page (width), and horizontally (height), respectively. It has two types of atoms and three types of bonds. The graph shown in Figure 3 is the three-dimensional sodalite network SOD (ḷ,ṃ,ṇ). Three different edge types and two different vertex types are present. There are $8(\text{ḷṃ}+\text{ḷṇ}+\text{ṃṇ})$ vertices of degree 3 and $12\text{ḷṃṇ}-4(\text{ḷṃ}+\text{ḷṇ}+\text{ṃṇ})$ vertices are of degree 4. It has a total of $12\text{ḷṃṇ}+4(\text{ḷṃ}+\text{ḷṇ}+\text{ṃṇ})$ vertices and $24\text{ḷṃṇ}+4(\text{ḷṃ}+\text{ḷṇ}+\text{ṃṇ})$ edges.

4. Main Results

In this section, we have computed some degree-based irregularity topological indices and reverse irregularity indices for SOD (ḷ,ṃ,ṇ) and the graph is depicted in Figure 3. The computational results are as follows.

Theorem 1. *Let the* **SOD** $(ḷ, ṃ, ṇ)$ *be the graph of sodalite materials network, then its irregularity indices are as follows:*

(1) $\mathrm{IRDIF}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 14/3\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(2) $AL(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 8\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(3) $\mathrm{IRL}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 2.3014\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(4) $\mathrm{IRLU}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 8/3\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(5) $\mathrm{IRLF}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 4/\sqrt{3}\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(6) $\mathrm{IRF}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 8\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(7) $\mathrm{IRLA}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 16/7\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(8) $\mathrm{IRD1}(\mathrm{SOD}(ḷ,ṃ,ṇ)) = 5.5451\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$
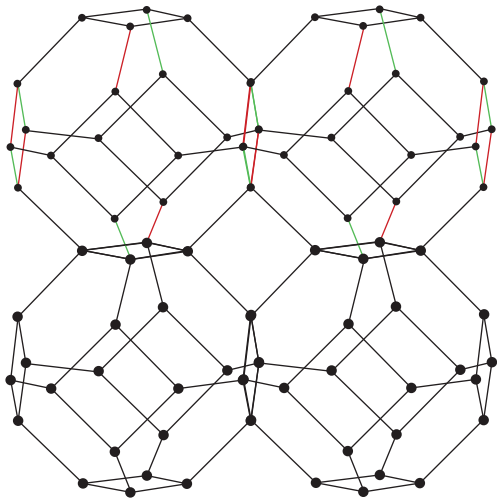
Figure 3: Sodalite materials network $\mathrm{SOD}(2,2,1)$.

(9) $\mathrm{IRA}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 0.478\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(10) $\mathrm{IRGA}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 0.0824\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(11) $\mathrm{IRB}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 0.5743\{(pq + \mathrm{pr} + qr) - (p+q+r)\}$

(12) $\mathrm{IRR_t}(\mathrm{SSOD}(ļ,ɱ,ŋ)) = 4\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

Proof. According to edge partition of $\mathrm{SOD}(ļ,ɱ,ŋ)$ given in Table 1 and above definitions, we computed the irregularity indices, and the computations are given by

(1) $\mathrm{IRDIF}(\mathrm{SOD}(ļ,ɱ,ŋ))) = \sum_{\mu v \in E(\mathbb{H})}|d_\mu/d_v - d_v/d_\mu| = |3/3 - 3/3|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |3/4 - 4/3|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |4/4 - 4/4|\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 0 + 7/12 \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} + 0 \ \mathrm{IRDIF}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 14/3\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(2) $\mathrm{AL}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}|d_\mu - d_v| = |3 - 3|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |3 - 4|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |4 - 4|\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} \mathrm{AL}(\mathrm{SOD}(ļ,ɱ,ŋ))) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(3) $\mathrm{IRL}(\mathrm{SOD}(ļ,ɱ,ŋ))) = \sum_{\mu v \in E(\mathbb{H})}|\ln d_\mu - \ln d_v| = |\ln 3 - \ln 3|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |\ln 3 - \ln 4|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |\ln 4 - \ln 4|\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 0.2876 \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} \mathrm{IRL}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 2.3014\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(4) $\mathrm{IRLU}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}|d_\mu - d_v|/\min(d_\mu, d_v) = |3 - 3|/3\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |3 - 4|/3\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |4 - 4|/4\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 1/2\{8(pq + \mathrm{pr} + qr) - 8(p + q + r)\} \mathrm{IRLU}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 8/3\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(5) $\mathrm{IRLF}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}|d_\mu - d_v|/\sqrt{d_\mu d_v} = |3 - 3|/\sqrt{9}\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |3 - 3|/\sqrt{12}\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |4 - 4|/\sqrt{16}\{24ļ ɱ ŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 8/2\sqrt{3}\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} \mathrm{IRLF}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 4/\sqrt{3}\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(6) $\mathrm{IRF}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}(d_\mu - d_v)^2 = (3 - 3)^2\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + (3 - 4)^2\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + (4 - 4)^2\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} \mathrm{IRF}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(7) $\mathrm{IRLA}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 2\sum_{\mu v \in E(\mathbb{H})}|d_\mu - d_v|/(d_\mu + d_v) = 2[|3 - 3|/(3 + 3)\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |3 - 4|/(3 + 4)\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |4 - 4|/(4 + 4)\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\}] = 2[8/7\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}] \mathrm{IRLA}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 16/7\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(8) $\mathrm{IRD1}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}\ln\{1 + |d_\mu - d_v|\} = \ln\{1 + |3 - 3|\}\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + \ln\{1 + |3 - 4|\}\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + \ln\{1 + |4 - 4|\}\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = \ln 2 \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} \mathrm{IRD1}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 5.5451\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(9) $\mathrm{IRA}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}(d_\mu^{-1/2} - d_v^{-1/2})^2 = (3^{-1/2} - 3^{-1/2})\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + (3^{-1/2} - 4^{-1/2})^2\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + (4^{-1/2} - 4^{-1/2})^2\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = (0.0773)^2\{8(pq + \mathrm{pr} + qr) - 8(p + q + r)\} = 0.0478\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(10) $\mathrm{IRGA}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}\ln((d_\mu + d_v)/2\sqrt{d_\mu d_v}) = \ln(3 + 3)/2\sqrt{9}\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + \ln(3 + 4)/2\sqrt{12}\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + \ln(4 + 4)/2\sqrt{16}\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = \ln 7/4\sqrt{3} \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} \mathrm{IRGA}(\mathrm{SSOD}(ļ,ɱ,ŋ)) = 0.0824\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(11) $\mathrm{IRB}(\mathrm{SOD}(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})}(\sqrt{d_\mu} - \sqrt{d_v})^2 = (\sqrt{3} - \sqrt{3})^2\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + (\sqrt{3} - \sqrt{4})^2\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + (\sqrt{4} - \sqrt{4})^2\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 0.07179 \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} \mathrm{IRB}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 0.5743\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(12) $\mathrm{IRR_t}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 1/2\sum_{\mu v \in E(\mathbb{H})}|d_\mu - d_v| = 1/2[|3 - 3|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |3 - 4|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |4 - 4|\{24ļɱŋ - 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\}] = 1/2 \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\} \mathrm{IRR_t}(\mathrm{SOD}(ļ,ɱ,ŋ)) = 4\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$ □

Theorem 2. *Let the* $\mathbf{SOD}(ļ, ɱ, ŋ)$ *be the graph of sodalite materials network, then its reverse irregularity indices are as follows:*

Table 1: Edge partition of sodalite materials network $SOD(ļ,ɱ,ŋ)$ on the degree of end vertices of each edge.

Types of edges	$(d_\mu, d_v), \mu v \in SOD(ļ,ɱ,ŋ)$	No.of edges/frequency
$E_1(3,3)$	$(3,3)$	$8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)$
$E_2(3,4)$	$(3,4)$	$8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)$
$E_3(4,4)$	$(4,4)$	$24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)$

Table 2: Numerical table of irregularity indices associated with the structure of $SOD(ļ,ɱ,ŋ)$ for different values of $ļ,ɱ,ŋ$.

$[ļ,ɱ,ŋ]$	$[2,2,2]$	$[3,3,3]$	$[4,4,4]$	$[5,5,5]$
$IRDIF(\mathbb{H})$	28	84	168	280
$AL(\mathbb{H})$	48	144	288	480
$IRL(\mathbb{H})$	13.8084	41.4252	82.8504	138.084
$IRLU(\mathbb{H})$	16	48	96	160
$IRLF(\mathbb{H})$	13.8564	41.5692	83.1384	138.5640
$IRF(\mathbb{H})$	48	144	288	480
$IRLA(\mathbb{H})$	13.7142	41.1428	82.2857	137.1428
$IRD1(\mathbb{H})$	33.2706	99.8118	199.6236	332.706
$IRA(\mathbb{H})$	0.2868	0.8604	1.7208	2.868
$IRGA(\mathbb{H})$	0.4944	1.4832	2.9664	4.944
$IRB(\mathbb{H})$	3.4458	10.3374	20.6748	34.458
$IRR_t(\mathbb{H})$	24	72	144	240

(1) $CIRDIF(SOD(ļ,ɱ,ŋ)) = 12\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(2) $CAL(SOD(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(3) $CIRL(SOD(ļ,ɱ,ŋ)) = 5.545\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(4) $CIRLU(SOD(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(5) $CIRLF(SOD(ļ,ɱ,ŋ)) = 8/\sqrt{2}\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(6) $CIRF(SOD(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(7) $CIRLA(SOD(ļ,ɱ,ŋ)) = 16/3\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(8) $CIRD1(SOD(ļ,ɱ,ŋ)) = 5.5451\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(9) $CIRA(SOD(ļ,ɱ,ŋ)) = 0.6862\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(10) $CIRGA(SOD(ļ,ɱ,ŋ)) = 0.4711\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(11) $CIRB(SOD(ļ,ɱ,ŋ)) = 1.3725\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(12) $CIRR_t(SOD(ļ,ɱ,ŋ)) = 4\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

Proof. According to edge partition of $SOD(ļ,ɱ,ŋ)$ given in Table 1 and above definitions, we computed the reverse irregularity indices, and the computations are given by

(1) $CIRDIF(SOD(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})} |(c_\mu/c_v) - c_v/c_\mu|$
$= |(2/2) - (2/2)|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |(2/1) - (1/2)|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |(1/1) - (1/1)|\{24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 0 + 3/2 \times 8\{(pq + pr + qr) - (p + q + r)\} + 0$
$CIRDIF(SOD(ļ,ɱ,ŋ)) = 12\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(2) $CAL(SOD(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})} |c_\mu - c_v| = |2 - 2|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |2 - 1|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |2 - 2|\{24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\}CAL(SOD(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(3) $CIRL(SOD(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})} |\ln c_\mu - \ln c_v| = |\ln 2 - \ln 2|\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |\ln 2 - \ln 1|\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |\ln 1 - \ln 1|\{24ļɱŋ- 12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 0.6931 \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}CIRL(SOD(ļ,ɱ,ŋ)) = 5.5451\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(4) $CIRLU(SOD(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})} (|c_\mu - c_v|/\min(c_\mu, c_v)) = (|2 - 2|/2)\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |2 - 1|/1\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |1 - 1|/1\{24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$ $CIRLU(SOD(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(5) $CIRLF(SOD(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})} |c_\mu - c_v|/\sqrt{c_\mu c_v} = |2 - 2|/\sqrt{4}\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + |2 - 1|/\sqrt{2}\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + |1 - 1|/\sqrt{1}\{24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} = 1/\sqrt{2} \times 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}CIRLF(SOD(ļ,ɱ,ŋ)) = 8/\sqrt{2}\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(6) $CIRF(SOD(ļ,ɱ,ŋ)) = \sum_{\mu v \in E(\mathbb{H})} (c_\mu - c_v)^2 = (2 - 2)^2\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + (2 - 1)^2\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + (1 - 1)^2\{24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\}CIRF(SOD(ļ,ɱ,ŋ)) = 8\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

(7) $CIRLA(SOD(ļ,ɱ,ŋ)) = 2\sum_{\mu v \in E(\mathbb{H})} |c_\mu - c_v|/(c_\mu + c_v) = 2[(|2 - 2|/(2 + 2))\{8(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\} + (|2 - 2|/(2 + 1))\{8(ļɱ+ļŋ+ɱŋ) - 8(ļ+ɱ+ŋ)\} + (|1 - 1|/(1 + 1))\{24ļɱŋ-12(ļɱ+ļŋ+ɱŋ) + 4(ļ+ɱ+ŋ)\}] = 2[8/3\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}]CIRLA(SOD(ļ,ɱ,ŋ)) = 16/3\{(ļɱ+ļŋ+ɱŋ) - (ļ+ɱ+ŋ)\}$

TABLE 3: Numerical table of reverse irregularity indices associated with the structure of SOD(ḷ,ṃ,ṇ) for different values of ḷ,ṃ,ṇ.

[ḷ, ṃ, ṇ]	[2, 2, 2]	[3, 3, 3]	[4, 4, 4]	[5, 5, 5]
CIRDIF (ℍ)	72	216	432	720
CAL (ℍ)	48	144	288	480
CIRL (ℍ)	33.2706	99.8118	199.6236	332.706
CIRLU (ℍ)	48	144	288	480
CIRLF (ℍ)	33.9411	101.8233	203.6467	339.4112
CIRF (ℍ)	48	144	288	480
CIRLA (ℍ)	32	96	192	320
CIRD1 (ℍ)	33.2706	99.8118	1996236	332.706
CIRA (ℍ)	4.1172	12..3516	24.7032	41172
CIRGA (ℍ)	2.8266	8.4798	16.9596	28.266
CIRB (ℍ)	8.235	24.705	49.41	82.35
CIRR$_t$ (ℍ)	24	72	144	240
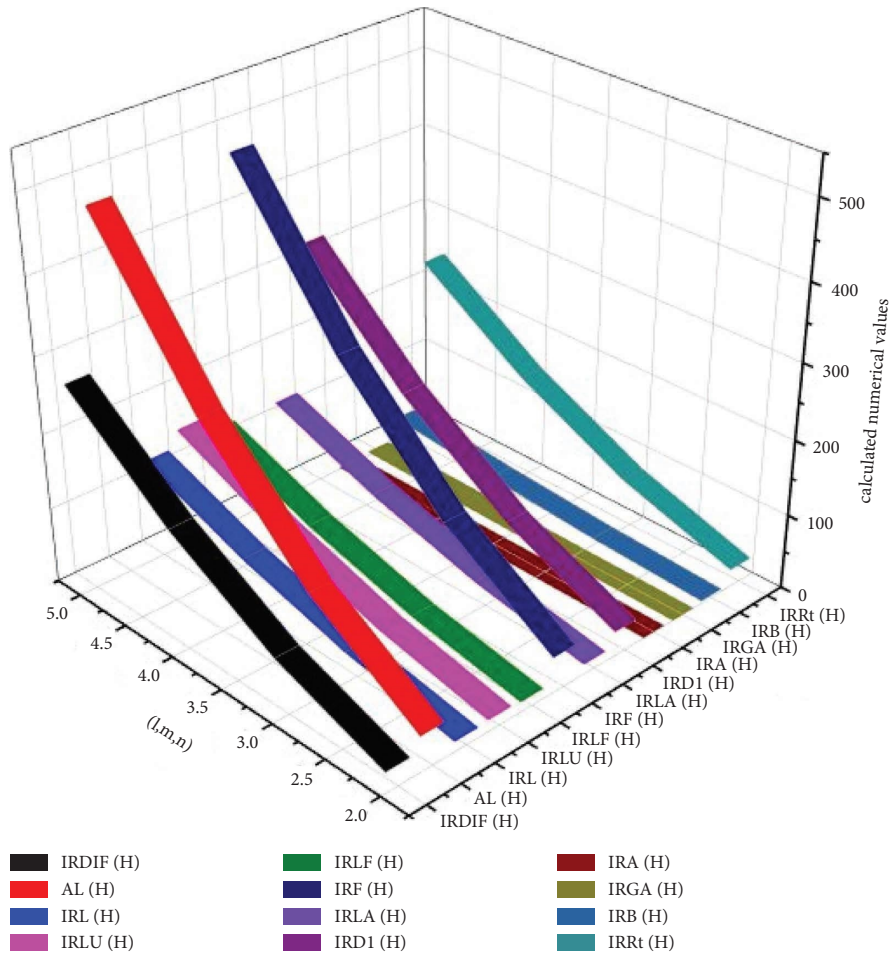
FIGURE 4: 3D graphical representation of Table 2.

(8) CIRD1 (SOD(ḷ,ṃ,ṇ)) $= \sum_{\mu v \in E(ℍ)}$ ln $\{1+ |c_\mu - c_v|\} =$ ln $\{1 + |2 - 2|\}\{8(ḷṃ+ḷ \quad ṇ+ṃṇ) + 4(ḷ+ṃ+ṇ)\}+$ ln $\{1 + |2 - 1|\}\{8(ḷṃ+ ḷṇ+ṃṇ) - 8(ḷ+ṃ+ṇ)\}+$ ln $\{1+ |1 - 1|\}\{24ḷṃṇ - 12(ḷṃ+ ḷṇ+ṃṇ) + 4 \quad (ḷ+ṃ +ṇ)\} =$ ln $2 \times 8\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$ CIRD1 (SOD(ḷ,ṃ,ṇ)) $= 5.5451 \quad \{(ḷṃ+ḷṇ+ \quad ṃṇ) - (ḷ+ ṃ+ṇ)\}$

(9) CIRA (SOD(ḷ,ṃ,ṇ)) $= \sum_{\mu v \in E(ℍ)} (c_\mu^{-1/2} - c_v^{-1/2})^2 =$ $(2^{-1/2} - 2^{-1/2})\{8(ḷṃ+ḷṇ+ṃṇ) + 4(ḷ+ṃ+ṇ)\} +$

$(2^{-1/2} - 1^{-1/2})^2\{8(ḷṃ+ḷṇ+ṃṇ) - 8(ḷ+ṃ+ṇ)\} +$ $(1^{-1/2} - 1^{-1/2})^2 \quad \{24ḷṃṇ - 12(ḷṃ+ḷṇ \quad +ṃṇ) + 4$ $(ḷ+ṃ+ ṇ)\} = 0.857\{8(ḷṃ+ ḷṇ+ṃṇ) - 8 \quad (ḷ+ṃ+ṇ)\}$ CIRA (SOD(ḷ,ṃ,ṇ)) $= 0.6862\{(ḷṃ+ḷṇ+ ṃṇ) - (ḷ+ ṃ+ṇ)\}$

(10) CIRGA (SOD(ḷ,ṃ,ṇ)) $= \sum_{\mu v \in E(ℍ)}$ ln $(c_\mu + c_v)/2$ $\sqrt{c_\mu c_v} =$ ln $(2 + 2)/2\sqrt{4}\{8(ḷṃ+ḷṇ+ṃṇ) + 4 \quad (ḷ+ ṃ+ ṇ)\} +$ ln $(2 + 1)/2\sqrt{2}\{8(ḷṃ+ḷṇ+ṃṇ) - 8(ḷ+ṃ+ṇ)\} +$ ln $(1 + 1)/2\sqrt{1}\{24ḷṃṇ - 12 \quad (ḷṃ+ḷṇ+ṃṇ) + 4 \quad (ḷ+$
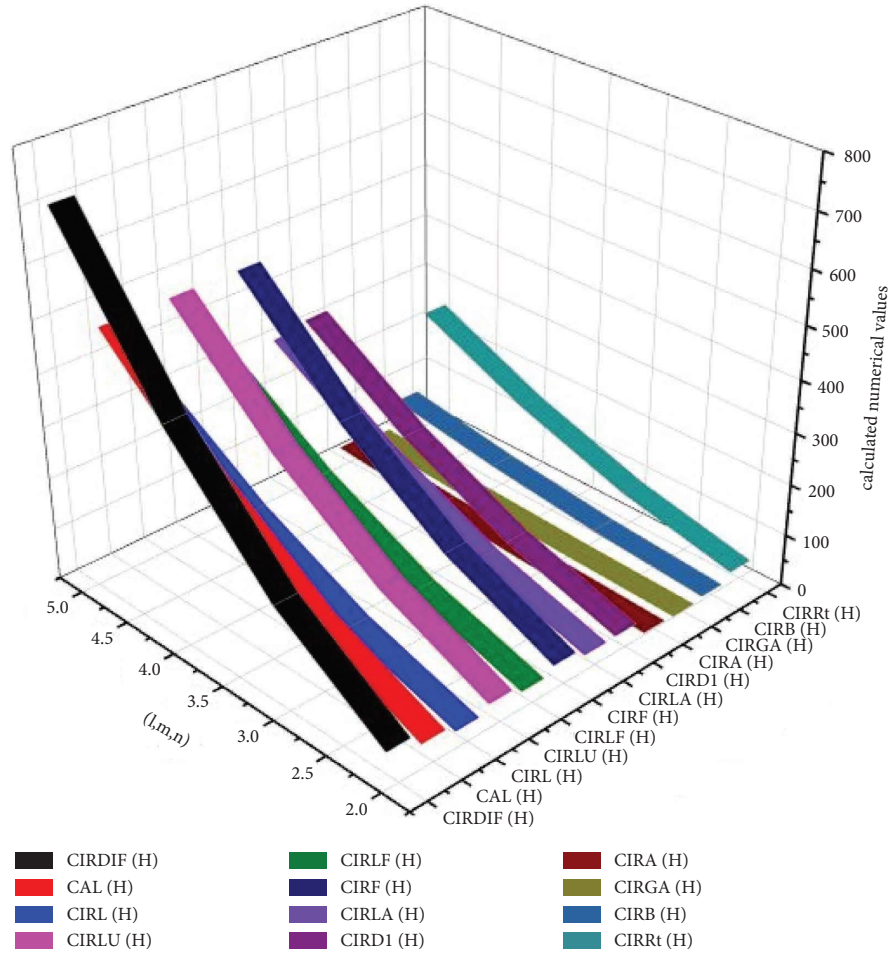
FIGURE 5: 3D graphical representation of Table 3.

$ṃ+ṇ)\} = \ln 3/2\sqrt{2} \times 8\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

$CIRGA(SOD(ḷ,ṃ,ṇ)) = 0.4711\{(ḷṃ+ ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

(11) $CIRB(SOD(ḷ,ṃ,ṇ)) = \sum_{\mu v \in E(\mathbb{H})}(\sqrt{c_\mu} - \sqrt{c_v})^2 = (\sqrt{2} - \sqrt{2})^2\{8(ḷṃ+ḷṇ+ ṃṇ) + 4 (ḷ+ṃ+ṇ)\} + (\sqrt{2} - \sqrt{1})^2\{8(ḷṃ+ḷṇ+ ṃṇ) - 8(ḷ+ ṃ+ṇ)\} + (\sqrt{1} - \sqrt{1})^2\{24ḷṃṇ - 12(ḷṃ+ḷṇ+ṃṇ) + 4 (ḷ+ ṃ+ṇ)\} = 0.1715 \times 8\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$

$CIRB(SOD(ḷ,ṃ,ṇ)) = 1.3725\{(ḷṃ+ ḷṇ+ṃṇ) - (ḷ+ ṃ+ṇ)\}$

(12) $CIRR_t(SOD(ḷ,ṃ,ṇ)) = (1/2)\sum_{\mu v \in E} (\mathbb{H})|c_\mu - c_v| = (1/2)[|2 - 2|\{8(ḷṃ+ḷṇ+ṃ ṇ) + 4(ḷ+ṃ+ ṇ)\} + |2 - 1|\{8(ḷṃ+ḷṇ+ṃṇ) - 8 (ḷ+ṃ+ṇ)\} + |1 - 1|\{24 ḷṃṇ - 12(ḷṃ+ ḷṇ+ṃṇ) + 4(ḷ+ṃ+ ṇ)\}] = 1/2 \times 8 \{(ḷṃ+ḷṇ+ṃ ṇ) - (ḷ+ṃ+ṇ)\}CIRR_t (SOD(ḷ,ṃ, ṇ))) = 4\{(ḷṃ+ḷṇ+ṃṇ) - (ḷ+ṃ+ṇ)\}$ □

5. Numerical Results and Concluding Remarks

In this study, we examined the sodalite material network, which is the most essential zeolite structure, and we showed the fetched graph of this network by $SOD(ḷ,ṃ,ṇ)$, defined in Figure 3 with parameters $ḷ,ṃ,ṇ \geq 1$. We calculated irregularity indices and reverse irregularity indices for the sodalite material network $SOD(ḷ,ṃ,ṇ)$. The numerical values of irregularity and reverse irregularity indices are shown in Tables 2 and 3, respectively, and Figures 4 and 5 show graphical comparisons. The strategic considerations of degree-based irregularity indices and reverse irregularity indices, in turn, refer as tools for predicting several properties of molecular compounds without laboratory experiments. These indices are useful in turning the molecular structure into a real number and predicting the main properties of chemical compounds. As a consequence, we anticipate that our findings could help forecast the varied features of zeolite systems. We also used graphical representations of the topological indices to explain our computed results. This research could serve as a model for future researchers looking to create new zeolites. Furthermore, we investigated the usefulness of these indices and discovered a substantial association when the parameters $ḷ,ṃ,ṇ$ increased in nature. From the analysis, we have developed numerical interpretations by comparing different values of $ḷ,ṃ,ṇ$. It is found that the AL index and IRF index are suitable for polarization, heavy atom count, molar refraction, and molar weight properties. It is natural and interesting to study the entropy measures and distance-based topological indices for sodalite materials. In the near future, firstly, we intend to find the entropy measures and distance-based topological indices for sodalite materials. Secondly, we aim to investigate the Szeged and Mostar root-indices of sodalite materials.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Authors' Contributions

The authors Shahid Zaman, Muhammad Salman, and Asad Ullah have equally contributed to this manuscript in all stages, from conceptualization to the write-up of final draft. Shahzad Ahmad and Mohammed Salaheldeen Abdelgader Abas contributed to methodology, analysis of results, and reviewing the final draft.

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