Research Article

M-Polynomials and Associated Topological Indices of Sodalite Materials

Ghazanfar Abbas,¹ Muhammad Ibrahim ,¹ Ali Ahmad ,² Muhammad Azeem ,³ and Kashif Elahi ⁴

¹Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan, Pakistan

²College of Computer Science & Information Technology, Jazan University, Jazan, Saudi Arabia

³Department of Aerospace Engineering, Faculty of Engineering, Universiti Putra Malaysia, Seri Kembangan, Malaysia

⁴Deanship of E-Learning and Information Technology, Jazan University, Jazan, Saudi Arabia

Correspondence should be addressed to Muhammad Ibrahim; mibtufail@gmail.com

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Natural zeolites are commonly described as macromolecular sieves. Zeolite networks are very trendy chemical networks due to their low-cost implementation. Sodalite network is one of the most studied types of zeolite networks. It helps in the removal of greenhouse gases. To study this rich network, we use an authentic mathematical tool known as M-polynomials of the topological index and show some physical and chemical properties in numerical form, and to understand the structure deeply, we compare different legitimate M-polynomials of topological indices, concluding in the form of graphical comparisons.

1. Introduction

Macromolecular sieves, commonly known as natural zeolites, are becoming more investigated and researched [1–3]. The custom-made molecular capturing of zeolite makes it significant and very applicable. Due to their lower costs, natural zeolites are considered as useful in bulk mineral applications [4]. According to the complexity and varying sizes, zeolites are characterized into different groups. For example, tschernichite, stilbite, mordenite, chabazite, faujasite, sodalite and Linde type A are most useful in terms of commercial applications, molecular sieves, or natural zeolites [5]. Among all the zeolite structures stated above, synthetic compounds and mineral's crystal structure with the frameworks of sodalite structure are the enormously studied compounds [6, 7]. Some physical and chemical properties of sodalite and zeolite type structures in terms of topological indices can be found in [8–10].

The sodalites with the highest thermodynamic stability are considered as one of the top ranked structures among all

the zeolites [11, 12]. The sodalites are also considerable due to their crystallographic standpoints [13]. The sodalite structure's unit cell is built up by two cages. The six and four membered rings represent the basic topology of each cage. These rings are also shared by two parallel cages. To trap the molecules, in the sodalite, cavities are built up by tailor-made composition. Without damaging the crystal structures, tap molecules like water and CO₂ have ability of desorbing and adsorbing molecules. As a result, for the removal of greenhouse gases and water, zeolites can be used [14]. For further studies related to zeolites, sodalite, and its useful applications, we refer the readers to [15, 16].

As we know that the study of M-polynomial is a very useful combination of numerical descriptors and algebraic theory, for the study of chemical networks, one can find an intense study on this topic; very particular and selected articles are cited here. Nanotube-related networks or structures were studied in [17–19], M-polynomials for different generalized families of graphs were discussed in [20–22], convex polytopes were studied in [23], chemical

benzenoid structures were discussed in [24], a fine relation of M-polynomial with the probabilistic theory was discussed in [25], the study of this topic on metal organic structure was detailed in [26, 27], and some computer-related networks in terms of M-polynomials can be found in [28, 29]; there are many types of polynomials, and one of the varieties can be found in [30].

Topological index is a function in numerical form and describes the biological, chemical, and physical properties of given molecular graph in domain by a systematic way. Few very interesting and highly recommended topological indices are given in the following definitions along with their M-polynomials. The researchers in [31] studied polyhex and prism structures in terms of some M-polynomials. The titania nanotubes were studied in terms of some M-polynomials in [32]. The structure of nanostar dendrimers and polyhex nanotubes was studied in [33]. For few interesting studies of chemical structures and their topological properties and different shapes, we refer the readers to [34, 35]. There are many ways and types of computing topological indices for different structures, for example, Shabbir et al. [36] computed the edge-based interpolation with the degree of vertices and topological indices, Nadeem et al. and Hong et al. [37, 38] computed the topological indices for the metal organic structure; line graph of some families of graphs and their topological indices are resulted in [39, 40], some ev- and ve-degree-based descriptors are studied in [41, 42], and the topological descriptors for some computer-related structures are discussed in [43, 44]. Some neural networks and their topological descriptors were discussed in [45, 46].

To compute our major results, we need to define some basics; for example, let χ be a graph with vertex set χ and edge set $E(\chi)$; their cardinalities are represented by n_χ and m_χ , respectively. Degree of a vertex (say λ_a) is the cardinality of incident edges with a vertex. There is another way to define edge set, which is called edge partition, usually written as (ξ_a, ξ_b) , where ξ_a, ξ_b are the degrees of vertices a and b , respectively, and a, b create an edge say ab .

Following are some useful definitions of M-polynomials which are helpful to find our main results and create formulas for M-polynomials of different topological indices.

Definition 1. In 1988, Hosoya polynomial was introduced in [47]; with a relevance to Hosoya polynomial, in 2015, modified polynomial or usually named as M-polynomial was given in [48]. This particular type of polynomial is closely related to degree-based topological indices. Using a particular type of format, one can get the topological indices from M-polynomials of a graph. This M-polynomial can be defined as

$$M(\chi; x, y) = \sum_{i \leq j} m_{i,j}(\chi) x^i y^j, \quad (1)$$

where $m_{i,j}(\chi)$ is the number of edges of graph χ such that $i \leq j$.

Definition 2. The first and second Zagreb indices were introduced in 1972 by Gutman [49, 50], and their M-polynomials are defined as [48]

$$\begin{aligned} M_1(\chi) &= \sum_{ab \in E(\chi)} (\xi_a + \xi_b), \\ M_2(\chi) &= \sum_{ab \in E(\chi)} (\xi_a \times \xi_b), \\ P_{M_1}(\chi) &= (D_x + D_y)(M(\chi; x, y)), \\ P_{M_2}(\chi) &= (D_x D_y)(M(\chi; x, y)). \end{aligned} \quad (2)$$

Definition 3. The second modified Zagreb index was given in [51], and its M-polynomial is defined as [48]

$$\begin{aligned} {}^m M_2 M_2(\chi) &= \sum_{ab \in E(\chi)} \frac{1}{\xi_a \times \xi_b}, \\ P_{{}^m M_2}(\chi) &= (S_x S_y)(M(\chi; x, y)). \end{aligned} \quad (3)$$

Definition 4. In 1988, Bollobas and Erdos and Amic et al. [52, 53] proposed the general Randić index independently. Following are general Randić index, general inverse Randić index, and their M-polynomials [48]:

$$\begin{aligned} R_\alpha(\chi) &= \sum_{uv \in E(\chi)} (\xi_u \times \xi_v)^\alpha, \\ P_{R_\alpha}(\chi) &= (D_x^\alpha D_y^\alpha)(M(\chi; x, y)), \\ IR_\alpha(\chi) &= \sum_{ab \in E(\chi)} \left(\frac{1}{\xi_a \times \xi_b} \right)^\alpha, \\ P_{IR_\alpha}(\chi) &= (S_x^\alpha S_y^\alpha)(M(\chi; x, y)), \end{aligned} \quad (4)$$

where

$$D_x(f(x, y)) = x \frac{\partial f}{\partial x}, \quad (5)$$

$$D_y(f(x, y)) = x \frac{\partial f}{\partial y},$$

$$S_x(f(x, y)) = \int_0^x \frac{f(z, y)}{z} dz, \quad (6)$$

$$S_y(f(x, y)) = \int_0^y \frac{f(x, z)}{z} dz. \quad (7)$$

In this research work, we studied sodalite's three-dimensional structure which is an important compound of zeolite network, in terms of different M-polynomials of topological indices defined above. Moreover, we explain the structure more precisely by taking different numerical examples and doing comparative study between computed M-polynomials, and at the end, we conclude the study in the form of graphical representations of derived numerical examples.

2. Results of M-Polynomials on Sodalite Network

The graph shown in Figure 1 is the three-dimensional sodalite network $S_{p,q,r}$. It contains $4(pq + pr + qr) + 12pqr$ total number of vertices and $4(pq + pr + qr) + 524pqr$ total number of edges. As shown in Figure 1, it contains two types of vertices and three types of edges, which are useful for our main results. Figure 1 is studied in [14] in detail to explore some useful structures related to sodalite and zeolites. Now, the first result is the main and general M-polynomial of sodalite network $S_{p,q,r}$.

Theorem 1. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, whose structure can be seen in Figure 1. Then, its M-polynomial is

$$\begin{aligned} M(S_{p,q,r}; x, y) &= 24pqr x^4 y^4 + 4(pq + pr + qr) \\ &\quad (2x^3 y^3 + 2x^3 y^4 - 3x^4 y^4) \\ &\quad + 4(p + q + r)(x^3 y^3 - 2x^3 y^4 + x^4 y^4). \end{aligned} \quad (8)$$

Proof. From Figure 1, which is the construction of sodalite materials, we can observe that there are two vertex set partitions:

$$\begin{aligned} V_3 &= \{\theta \in V(S_{p,q,r}) : d_\theta = 3\}, \\ V_4 &= \{\theta \in V(S_{p,q,r}) : d_\theta = 4\}, \end{aligned} \quad (9)$$

with $|V_3| = 8(pq + pr + qr)$ and $|V_4| = 12pqr - 4(pq + pr + qr)$. Also, there are three edge partitions based on degree of end vertices of each edge that is defined as

$$\begin{aligned} \Xi_{3,3} &= \{\theta\lambda \in E(S_{p,q,r}) : d_\theta = 3, d_\lambda = 3\}, \\ \Xi_{3,4} &= \{\theta\lambda \in E(S_{p,q,r}) : d_\theta = 3, d_\lambda = 4\}, \\ \Xi_{4,4} &= \{\theta\lambda \in E(S_{p,q,r}) : d_\theta = 4, d_\lambda = 4\}. \end{aligned} \quad (10)$$

The cardinality of these edge partitions is $m_{3,3} = |\Xi_{3,3}| = 8(pq + pr + qr) + 4(p + q + r)$, $m_{3,4} = |\Xi_{3,4}| = 8(pq + pr + qr) - 8(p + q + r)$, and $m_{4,4} = |\Xi_{4,4}| = 24pqr - 12(pq + pr + qr) + 4(p + q + r)$. Then, from Definition 1, the M-polynomial of $S_{p,q,r}$ is

$$\begin{aligned} M(S_{p,q,r}; x, y) &= \sum_{i \leq j} m_{i,j}(S_{p,q,r}) x^i y^j \\ &= m_{3,3}(S_{p,q,r}) x^3 y^3 + m_{3,4}(S_{p,q,r}) x^3 y^4 \\ &\quad + m_{4,4}(S_{p,q,r}) x^4 y^4 \\ &= 24pqr x^4 y^4 + 4(pq + pr + qr) \\ &\quad (2x^3 y^3 + 2x^3 y^4 - 3x^4 y^4) \\ &\quad + 4(p + q + r)(x^3 y^3 - 2x^3 y^4 + x^4 y^4). \quad \square \end{aligned} \quad (11)$$

Lemma 1. Let $S_{4,4,4}$ be a sodalite material, with $p, q, r \geq 1$. Then, the differential operator is

$$\begin{aligned} D_x &= 96pqr x^4 y^4 + 24(pq + pr + qr) \\ &\quad \cdot (x^3 y^3 + x^3 y^4 - 2x^4 y^4) \\ &\quad + 4(p + q + r)(3x^3 y^3 - 6x^3 y^4 + 4x^4 y^4), \\ D_y &= 96pqr x^4 y^4 + 8(pq + pr + qr) \\ &\quad \cdot (3x^3 y^3 + 4x^3 y^4 - 6x^4 y^4) \\ &\quad + 4(p + q + r)(3x^3 y^3 - 8x^3 y^4 + 4x^4 y^4). \end{aligned} \quad (12)$$

Proof. Differentiating equation (8) with respect to x and multiplying the result with x , we get D_x . Similarly, differentiating equation (8) with respect to y and multiplying the result with y , we get D_y . $\square$

Lemma 2. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$. Then, the integral operator is

$$\begin{aligned} S_x &= 6pqr x^4 y^4 + 4(pq + pr + qr) \\ &\quad \cdot \left(\frac{2}{3} x^3 y^3 + \frac{2}{3} x^3 y^4 - \frac{3}{4} x^4 y^4 \right) \\ &\quad + 4(p + q + r) \left(\frac{1}{3} x^3 y^3 - \frac{2}{3} x^3 y^4 + \frac{1}{4} x^4 y^4 \right), \\ S_y &= 6pqr x^4 y^4 + 4(pq + pr + qr) \\ &\quad \cdot \left(\frac{2}{3} x^3 y^3 + \frac{1}{2} x^3 y^4 - \frac{3}{4} x^4 y^4 \right) \\ &\quad + 4(p + q + r) \left(\frac{1}{3} x^3 y^3 - \frac{1}{2} x^3 y^4 + \frac{1}{4} x^4 y^4 \right). \end{aligned} \quad (13)$$

Proof. As we know from equation (6), $S_x = \int_0^x (M(S_{p,q,r}; t, y)/t) dt$ and using the general M-polynomial for the $S_{p,q,r}$ from equation (8) in it, after simplification, we obtain S_x . Similarly, from equation (7), $S_y = \int_0^y (M(S_{p,q,r}; x, t)/t) dt$ and using the general M-polynomial for the $S_{p,q,r}$ from equation (8) in it, after simplification, we obtain S_y .

Now, we will use these differential and integral operators from Lemmas 1 and 2 to obtain our main results. In the following theorem, we determined the M-polynomial of first and second Zagreb indices.

Theorem 2. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and P_{M_1} be the M-polynomial of first Zagreb index. Then, $P_{M_1}(S_{p,q,r})$ is

FIGURE 1: Sodalite network.

$$\begin{aligned}
 P_{M_1}(S_{p,q,r}) &= 192pqr x^4 y^4 + 8(pq + pr + qr)(6x^3 y^3 + 7x^3 y^4 - 12x^4 y^4) \\
 &\quad + 8(p + q + r)(3x^3 y^3 - 7x^3 y^4 + 4x^4 y^4), \\
 P_{M_2}(S_{p,q,r}) &= 384pqr x^4 y^4 + 24(pq + pr + qr)(3x^3 y^3 + 4x^3 y^4 - 8x^4 y^4) \\
 &\quad + 4(p + q + r)(9x^3 y^3 - 24x^3 y^4 + 16x^4 y^4).
 \end{aligned} \tag{14}$$

Proof. According to Definition 2, the formula for the M-polynomial of first Zagreb index for $S_{p,q,r}$ is defined as $P_{M_1}(S_{p,q,r}) = (D_x + D_y)(M(S_{p,q,r}; x, y))$, by using the

differential operators that are defined in Lemma 1 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M-polynomial of first Zagreb index for $S_{p,q,r}$ as follows:

$$P_{M_1}(S_{p,q,r}) = 192pqr x^4 y^4 + 8(pq + pr + qr)(6x^3 y^3 + 7x^3 y^4 - 12x^4 y^4) + 8(p + q + r)(3x^3 y^3 - 7x^3 y^4 + 4x^4 y^4). \tag{15}$$

Similarly, by using the values of differential operators that are defined in Lemma 1 for $S_{p,q,r}$ in $P_{M_2}(S_{p,q,r})$

$= (D_x D_y)(M(S_{p,q,r}; x, y))$ and after simplification, we will get the M-polynomial of second Zagreb index for $S_{p,q,r}$:

$$P_{M_2}(S_{p,q,r}) = 384pqr x^4 y^4 + 24(pq + pr + qr)(3x^3 y^3 + 4x^3 y^4 - 8x^4 y^4) + 4(p + q + r)(9x^3 y^3 - 24x^3 y^4 + 16x^4 y^4). \tag{16}$$

Theorem 3. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and $P_{m_{M_2}}$ be the M-polynomial of second modified Zagreb index. Then, $P_{m_{M_2}}(S_{p,q,r})$ is

$$\begin{aligned}
 P_{m_{M_2}}(S_{p,q,r}) &= \frac{3}{2}pqr x^4 y^4 + 4(pq + pr + qr)\left(\frac{2}{9}x^3 y^3 + \frac{1}{8}x^3 y^4 - \frac{3}{16}x^4 y^4\right) \\
 &\quad + 4(p + q + r)\left(\frac{1}{9}x^3 y^3 - \frac{1}{8}x^3 y^4 + \frac{1}{16}x^4 y^4\right).
 \end{aligned} \tag{17}$$

Proof. According to Definition 3, the formula for the M-polynomial of second modified Zagreb index for $S_{p,q,r}$ is defined as $P_{m_{M_2}}(S_{p,q,r}) = (S_x S_y)(M(S_{p,q,r}; x, y))$, by using

the integral operators that are defined in Lemma 2 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M-polynomial of second modified Zagreb index for $S_{p,q,r}$ as

$$P_{mM_1}(S_{p,q,r}) = \frac{3}{2} pqr x^4 y^4 + 4(pq + pr + qr) \left(\frac{2}{9} x^3 y^3 + \frac{1}{8} x^3 y^4 - \frac{3}{16} x^4 y^4 \right) + 4(p + q + r) \left(\frac{1}{9} x^3 y^3 - \frac{1}{8} x^3 y^4 + \frac{1}{16} x^4 y^4 \right). \quad (18)$$

Theorem 4. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and P_{R_α} be the M -polynomial of general Randić index. Then, $P_{R_\alpha}(S_{p,q,r})$ is

$$P_{R_\alpha}(S_{p,q,r}) = 16^\alpha \times 24 pqr x^4 y^4 + 4(pq + pr + qr) (9^\alpha \times 2x^3 y^3 + 12^\alpha \times 2x^3 y^4 - 16^\alpha \times 3x^4 y^4) + 4(pq + pr + qr) (9^\alpha x^3 y^3 - 12^\alpha \times 2x^3 y^4 + 16^\alpha x^4 y^4). \quad (19)$$

Proof. According to Definition 4, the formula for the M -polynomial of general Randić index for $S_{p,q,r}$ is defined as $P_{R_\alpha}(S_{p,q,r}) = (D_x^\alpha D_y^\alpha)(M(S_{p,q,r}; x, y))$, by using the

differential operators that are defined in Lemma 1 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M -polynomial of general Randić index for $S_{p,q,r}$ as

$$P_{R_\alpha}(S_{p,q,r}) = 16^\alpha \times 24 pqr x^4 y^4 + 4(pq + pr + qr) (9^\alpha \times 2x^3 y^3 + 12^\alpha \times 2x^3 y^4 - 16^\alpha \times 3x^4 y^4) + 4(p + q + r) (9^\alpha x^3 y^3 - 12^\alpha \times 2x^3 y^4 + 16^\alpha x^4 y^4). \quad (20)$$

Theorem 5. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and P_{IR_α} be the M -polynomial of general inverse Randić index. Then, $P_{IR_\alpha}(S_{p,q,r})$ is

$$P_{IR_\alpha}(S_{p,q,r}) = \frac{24}{16^\alpha} pqr x^4 y^4 + 4(pq + pr + qr) \left(\frac{2}{9^\alpha} x^3 y^3 + \frac{2}{12^\alpha} x^3 y^4 - \frac{3}{16^\alpha} x^4 y^4 \right) + 4(p + q + r) \left(\frac{1}{9^\alpha} x^3 y^3 - \frac{2}{12^\alpha} x^3 y^4 + \frac{1}{16^\alpha} x^4 y^4 \right). \quad (21)$$

Proof. According to Definition 4, the formula for the M -polynomial of general inverse Randić index for $S_{p,q,r}$ is defined as $P_{IR_\alpha}(S_{p,q,r}) = (S_x^\alpha S_y^\alpha)(M(S_{p,q,r}; x, y))$, by using

the integral operators that are defined in Lemma 2 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M -polynomial of general inverse Randić index for $S_{p,q,r}$ as

$$P_{IR_\alpha}(S_{p,q,r}) = \frac{24}{16^\alpha} pqr x^4 y^4 + 4(pq + pr + qr) \left(\frac{2}{9^\alpha} x^3 y^3 + \frac{2}{12^\alpha} x^3 y^4 - \frac{3}{16^\alpha} x^4 y^4 \right) + 4(p + q + r) \left(\frac{1}{9^\alpha} x^3 y^3 - \frac{2}{12^\alpha} x^3 y^4 + \frac{1}{16^\alpha} x^4 y^4 \right). \quad (22)$$

3. Results of Topological Indices from M -Polynomials on Sodalite Materials

Lemma 3. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$. Then,

$$\begin{aligned} [D_x]_{(x,y)=(1,1)} &= 96pqr + 4(p + q + r), \\ [D_y]_{(x,y)=(1,1)} &= 96pqr + 8(pq + pr + qr) - 4(p + q + r). \end{aligned} \quad (23)$$

Proof. Differentiating equation (8) with respect to x and multiplying the result with x , we get D_x . Similarly, differentiating equation (8) with respect to y and multiplying the result with y , we get D_y . After that in both equations, substituting $(x, y) = (1, 1)$ and simplifying, we can easily obtain $[D_x]_{(x,y)=(1,1)}$ and $[D_y]_{(x,y)=(1,1)}$. $\square$

Lemma 4. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$. Then,

$$\begin{aligned}
[S_x]_{(x,y)=(1,1)} &= 6pqr + \frac{7}{3}(pq + pr + qr) - \frac{1}{3}(p + q + r), \\
[S_y]_{(x,y)=(1,1)} &= 6pqr + \frac{5}{3}(pq + pr + qr) + \frac{1}{3}(p + q + r).
\end{aligned}
\tag{24}$$

Proof. By putting the value of general M-polynomial which is defined in equation (8) in equation (6), after simplification, we get S_x . Similarly, by putting the value of general M-polynomial in equation (7), after simplification, we get S_y . After simplification, we obtain S_y . After that, in both equations, substituting $(x, y) = (1, 1)$ and simplifying, we can easily obtain $[S_x]_{(x,y)=(1,1)}$ and $[S_y]_{(x,y)=(1,1)}$. $\square$

Now, we will use these absolute values from the differential and integral operators which are from Lemmas 3 and 4 to obtain our main results. In the following theorem, we determined the topological indices from M-polynomial of first and second Zagreb indices.

Theorem 6. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and M_1, M_2 be the first and second Zagreb indices. Then, $M_1(S_{p,q,r})$ and $M_2(S_{p,q,r})$ are

$$\begin{aligned}
M_1(S_{p,q,r}) &= 192pqr + 8(pq + pr + qr), \\
M_2(S_{p,q,r}) &= 384pqr - 24(pq + pr + qr) + 4(p + q + r).
\end{aligned}
\tag{25}$$

Proof. According to Definition 2, the formula for the M-polynomial of first Zagreb index for $S_{p,q,r}$ is defined as $P_{M_1}(S_{p,q,r}) = (D_x + D_y)(M(S_{p,q,r}; x, y))$, by using the differential operators that are defined in Lemma 1 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M-polynomial of first Zagreb index for $S_{p,q,r}$.

Now using Lemma 3 and evaluating it in Definition 2 and after some algebraic simplifications, we will get the first Zagreb index for $S_{p,q,r}$ as

$$M_1(S_{p,q,r}) = 192pqr + 8(pq + pr + qr). \tag{26}$$

Similarly, by using the absolute values of differential operators that are defined in Lemma 3 for $S_{p,q,r}$ in $P_{M_2}(S_{p,q,r}) = (D_x D_y)(M(S_{p,q,r}; x, y))$ and after simplification, we will get the second Zagreb index for $S_{p,q,r}$:

$$M_2(S_{p,q,r}) = 384pqr - 24(pq + pr + qr) + 4(p + q + r). \tag{27}$$

Theorem 7. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and ${}^m M_2$ be the second modified Zagreb index. Then, ${}^m M_2(S_{p,q,r})$ is

$${}^m M_2(S_{p,q,r}) = \frac{3}{2}pqr + \frac{23}{36}(pq + pr + qr) + \frac{7}{36}(p + q + r). \tag{28}$$

Proof. According to Definition 3, the formula for the M-polynomial of second modified Zagreb index for $S_{p,q,r}$ is defined as ${}^m M_2(S_{p,q,r}) = (S_x S_y)(M(S_{p,q,r}; x, y))$, by using the integral operators that are defined in Lemma 2 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M-polynomial of second modified Zagreb index for $S_{p,q,r}$.

Now using Lemma 4 and evaluating it in Definition 3 and after some algebraic simplifications, we will get the modified Zagreb index for $S_{p,q,r}$ as

$$\{{}^m M_1\}(S_{p,q,r}) = \frac{3}{2}pqr + \frac{23}{36}(pq + pr + qr) + \frac{7}{36}(p + q + r). \tag{29}$$

Theorem 8. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and R_α be the general Randić index; then, $R_\alpha(S_{p,q,r})$ is

$$\begin{aligned}
R_\alpha(S_{p,q,r}) &= 16^\alpha \times 24pqr + 4(pq + pr + qr) \\
&\quad (9^\alpha \times 2 + 12^\alpha \times 2 - 16^\alpha \times 3) \\
&\quad + 4(pq + pr + qr)(9^\alpha - 12^\alpha \times 2 + 16^\alpha).
\end{aligned}
\tag{30}$$

Proof. According to Definition 4, the formula for the M-polynomial of general Randić index for $S_{p,q,r}$ is defined as $R_\alpha(S_{p,q,r}) = (D_x^\alpha D_y^\alpha)(M(S_{p,q,r}; x, y))$, by using the differential operators that are defined in Lemma 1 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M-polynomial of general Randić index for $S_{p,q,r}$.

Now using Lemma 3 and evaluating it in Definition 4 and after some algebraic simplifications, we will get the general Randić index for $S_{p,q,r}$ as

$$\begin{aligned}
R_\alpha(S_{p,q,r}) &= 16^\alpha \times 24pqr + 4(pq + pr + qr) \\
&\quad \cdot (9^\alpha \times 2 + 12^\alpha \times 2 - 16^\alpha \times 3) \\
&\quad + 4(pq + pr + qr)(9^\alpha - 12^\alpha \times 2 + 16^\alpha).
\end{aligned}
\tag{31}$$

Theorem 9. Let $S_{p,q,r}$ be a sodalite material, with $p, q, r \geq 1$, and R_α be the general inverse Randić index; then, $IR_\alpha(S_{p,q,r})$ is

$$\begin{aligned}
IR_\alpha(S_{p,q,r}) &= \frac{24}{16^\alpha}pqr + 4(pq + pr + qr)\left(\frac{2}{9^\alpha} + \frac{2}{12^\alpha} - \frac{3}{16^\alpha}\right) \\
&\quad + 4(p + q + r)\left(\frac{1}{9^\alpha} - \frac{2}{12^\alpha} + \frac{1}{16^\alpha}\right).
\end{aligned}
\tag{32}$$

Proof. According to Definition 4, the formula for the M-polynomial of general inverse Randić index for $S_{p,q,r}$ is defined as $IR_\alpha(S_{p,q,r}) = (S_x^\alpha S_y^\alpha)(M(S_{p,q,r}; x, y))$, by using the

FIGURE 2: General M-polynomial for three-dimensional sodalite network $S_{4,4,4}$.

FIGURE 5: Modified Zagreb M-polynomial for three-dimensional sodalite network $S_{4,4,4}$.

FIGURE 3: First Zagreb M-polynomial for three-dimensional sodalite network $S_{4,4,4}$.

FIGURE 6: General Randić M-polynomial for three-dimensional sodalite network $S_{4,4,4}$ and $\alpha = -(1/2)$.

FIGURE 4: Second Zagreb M-polynomial for three-dimensional sodalite network $S_{4,4,4}$.

FIGURE 7: General inverse Randić M-polynomial for three-dimensional sodalite network $S_{4,4,4}$ and $\alpha = -(1/2)$.

FIGURE 8: Contour plot of topological indices for three-dimensional sodalite network $S_{p,q,r}$ and $\alpha = -(1/2)$.

FIGURE 9: Topological indices for three-dimensional sodalite network $S_{p,q,r}$ and $\alpha = -(1/2)$.

integral operators that are defined in Lemma 2 for $S_{p,q,r}$. After some algebraic simplifications, we will get the M-polynomial of general inverse Randić index for $S_{p,q,r}$.

Now using Lemma 4 and evaluating it in Definition 4 and after some algebraic simplifications, we will get the general inverse Randić index for $S_{p,q,r}$ as

$$\begin{aligned} \text{IR}_\alpha(S_{p,q,r}) = & \frac{24}{16^\alpha} pqr + 4(pq + pr + qr) \left(\frac{2}{9^\alpha} + \frac{2}{12^\alpha} - \frac{3}{16^\alpha} \right) \\ & + 4(p + q + r) \left(\frac{1}{9^\alpha} - \frac{2}{12^\alpha} + \frac{1}{16^\alpha} \right). \end{aligned} \quad (33)$$

4. Conclusion and Discussion

In this study, we discussed the most important structure from zeolite structures which is known as sodalite material network and we symbolized the fetched graph of this network by $S_{p,q,r}$, defined in Figure 1. The moving parameters for this structure are $p, q, r \geq 1$. We study this structure for all these parameters in terms of different M-polynomials and topological indices derived from resulting M-polynomials. Figures 2–7 show the three-dimensional plot of resulting M-polynomials of first, second, and modified Zagreb M-polynomials and general and general inverse Randić M-polynomials, respectively. Figure 8 shows the contour plot of topological index derived from M-polynomials while Figure 9 shows the plot of all the topological indices derived from M-polynomials.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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