Research Article

M-Polynomials and Associated Topological Indices of Sodalite Materials

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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 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 [28], a finer relation of M-polynomial with the probabilistic theory was discussed in [29]. The topological structures were discussed in [24], a finer relation of M-polynomial with the probabilistic theory was discussed in [29]. The topological structures were discussed in [24], a finer relation of M-polynomial with the probabilistic theory was discussed in [29].

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

\[ M(\chi; x, y) = \sum_{i\leq j} m_{i, j}(\chi)x^i y^j, \]  

(1)

where \( m_{i, j}(\chi) \) is the number of edges of graph \( \chi \) 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]

\[ M_1(\chi) = \sum_{a\neq b} (\xi_a + \xi_b), \]

\[ M_2(\chi) = \sum_{a\neq b} (\xi_a \times \xi_b), \]  

(2)

\[ P_{M_1}(\chi) = \left(D_x + D_y\right)(M(\chi; x, y)), \]

\[ P_{M_2}(\chi) = \left(D_x D_y\right)(M(\chi; x, y)). \]

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

\[ M_2^m(\chi) = \sum_{a\neq b} \frac{1}{\xi_a \times \xi_b}, \]  

(3)

\[ P_{M_2^m}(\chi) = \left(S_x S_y\right)(M(\chi; x, y)). \]

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]:

\[ R_a(\chi) = \sum_{uv \in E(\chi)} (\xi_a \times \xi_b)^a, \]

\[ P_{R_a}(\chi) = \left(D_x^a D_y^a\right)(M(\chi; x, y)), \]  

(4)

\[ I_{R_a}(\chi) = \sum_{a\neq b} \frac{1}{\xi_a \times \xi_b} \]

\[ P_{I_{R_a}}(\chi) = \left(S_x^{ae} S_y^{ae}\right)(M(\chi; x, y)), \]

where

\[ D_x(f(x, y)) = \frac{\partial f}{\partial x}, \]

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

(5)

\[ S_x(f(x, y)) = \int_0^x f(z, y) \, dz, \]

\[ S_y(f(x, y)) = \int_0^y f(x, z) \, dz. \]  

(6)

(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 $S_{pqr}$. It contains $4(pq + pr + qr) + 12pqr$ total number of vertices and $4(pq + pr + qr) + 24pqr$ 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 $S_{pqr}$.

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

$$M(S_{pqr}, x, y) = 24pqr(x^3y^4 + 4(pq + pr + qr) \left(2x^3y^3 + 2x^3y^4 - 3x^4y^4\right) + 4(p + q + r)\left(x^3y^3 - 2x^3y^4 + x^4y^4\right)).$$

(8)

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

$$\mathcal{V}_3 = \{\theta \in V(S_{pqr}) : d_{\theta} = 3\},$$

$$\mathcal{V}_4 = \{\theta \in V(S_{pqr}) : d_{\theta} = 4\},$$

with $|\mathcal{V}_3| = 8(pq + pr + qr)$ and $|\mathcal{V}_4| = 24pqr - 4(pq + pr + qr)$. Also, there are three edge partitions based on degree of end vertices of each edge that is defined as

$$\mathcal{E}_{3,3} = \{\theta \in E(S_{pqr}) : d_{\theta} = 3, d_{\theta} = 3\},$$

$$\mathcal{E}_{3,4} = \{\theta \in E(S_{pqr}) : d_{\theta} = 3, d_{\theta} = 4\},$$

$$\mathcal{E}_{4,4} = \{\theta \in E(S_{pqr}) : d_{\theta} = 4, d_{\theta} = 4\}.$$

(10)

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

$$M(S_{pqr}; x, y)^{j} y^{j} = \sum_{i,j} m_{i,j}(S_{pqr}) x^{i} y^{j}$$

$$= m_{3,3}(S_{pqr}) x^{3} y^{3} + m_{3,4}(S_{pqr}) x^{3} y^{4}$$

$$+ m_{4,4}(S_{pqr}) x^{4} y^{4}$$

$$= 24pqr(x^3y^4 + 4(pq + pr + qr) \left(2x^3y^3 + 2x^3y^4 - 3x^4y^4\right) + 4(p + q + r)\left(x^3y^3 - 2x^3y^4 + x^4y^4\right))$$

(11)

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

$$D_x = 96pqrx^4y^4 + 24(pq + pr + qr) \left(x^3y^3 + x^3y^4 - 2x^4y^4\right)$$

$$+ 4(p + q + r)\left(3x^3y^3 - 6x^3y^4 + 4x^4y^4\right),$$

$$D_y = 96pqrx^4y^4 + 8(pq + pr + qr) \left(x^3y^3 + 4x^3y^4 - 6x^4y^4\right)$$

$$+ 4(p + q + r)\left(3x^3y^3 - 8x^3y^4 + 4x^4y^4\right).$$

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

$$S_x = 6pqrx^4y^4 + 4(pq + pr + qr) \left(\frac{2}{3}x^3y^3 + \frac{2}{3}x^3y^4 - \frac{3}{4}x^4y^4\right)$$

$$+ 4(p + q + r)\left(\frac{1}{3}x^3y^3 - \frac{2}{3}x^3y^4 + \frac{1}{4}x^4y^4\right),$$

$$S_y = 6pqrx^4y^4 + 4(pq + pr + qr) \left(\frac{2}{3}x^3y^3 + \frac{2}{3}x^3y^4 - \frac{3}{4}x^4y^4\right)$$

$$+ 4(p + q + r)\left(\frac{1}{3}x^3y^3 - \frac{1}{2}x^3y^4 + \frac{1}{4}x^4y^4\right).$$

(13)

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

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 $S_{pqr}$ be a sodalite material, with $p, q, r \geq 1$, and $P_M$, be the M-polynomial of first Zagreb index. Then, $P_{M_1}(S_{pqr})$ is
\[ P_{M_1}(S_{p,q,r}) = 192pqrx^4y^4 + 8(pq + pr + qr)(6x^3y^3 + 7x^3y^4 - 12x^4y^4) \]
\[ + 8(p + q + r)(3x^3y^3 - 7x^3y^4 + 4x^4y^4). \tag{14} \]

\[ P_{M_1}(S_{p,q,r}) = 384pqrx^4y^4 + 24(pq + pr + qr)(3x^3y^3 + 4x^3y^4 - 8x^4y^4) \]
\[ + 4(p + q + r)(9x^3y^3 - 24x^3y^4 + 16x^4y^4). \tag{15} \]

**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:

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

Similarly, by using the values of differential operators that are defined in Lemma 1 for \( S_{p,q,r} \) in \( P_{M_1}(S_{p,q,r}) = (D_x + D_y)(M(S_{p,q,r}; x, y)) \) and after simplification, we will get the M-polynomial of second Zagreb index for \( S_{p,q,r} \):

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

**Theorem 3.** Let \( S_{p,q,r} \) be a sodalite material, with \( p, q, r \geq 1 \), and \( P_{n_{M_1}} \) be the M-polynomial of second modified Zagreb index. Then, \( P_{n_{M_1}}(S_{p,q,r}) \) is

\[ P_{n_{M_1}}(S_{p,q,r}) = \frac{3}{2}pqrx^4y^4 + 4(pq + pr + qr)(\frac{2}{9}x^3y^3 + \frac{1}{8}x^3y^4 - \frac{3}{16}x^4y^4) \]
\[ + 4(p + q + r)\left(\frac{1}{9}x^3y^3 - \frac{1}{8}x^3y^4 + \frac{1}{16}x^4y^4\right). \tag{17} \]

**Proof.** According to Definition 3, the formula for the M-polynomial of second modified Zagreb index for \( S_{p,q,r} \) is defined as \( P_{n_{M_1}}(S_{p,q,r}) = (S_xS_y)(M(S_{p,q,r}; x, y)) \), 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...
\[ P_{M_1}(S_{p,q,r}) = \frac{3}{2} pqr x^4 y^4 + 4(p + pr + qr)(\frac{2}{9} x^3 y^3 + \frac{1}{8} x^3 y^4 - \frac{3}{16} x^4 y^4) + 4(p + q + r)(\frac{1}{9} x^3 y^3 - \frac{1}{8} x^3 y^4 + \frac{1}{16} x^4 y^4). \]  

(18)

**Theorem 4.** Let \( S_{p,q,r} \) be a sodalite material, with \( p, q, r \geq 1 \), and \( P_{M_1} \) be the M-polynomial of general Randić index. Then, \( P_{M_1}(S_{p,q,r}) \) is

\[ P_{M_1}(S_{p,q,r}) = 16^a \times 24 pqr x^4 y^4 + 4(p + pr + qr)(9^a \times 2x^3 y^3 + 12^a \times 2x^3 y^4 - 16^a \times 3x^4 y^4) + 4(p + q + r)(9^a x^3 y^3 - 12^a \times 2x^3 y^4 + 16^a x^4 y^4). \]  

(19)

**Proof.** According to Definition 4, the formula for the M-polynomial of general Randić index for \( S_{p,q,r} \) is defined as \( P_{M_1}(S_{p,q,r}) = (D_x^p D_y^q)(M(S_{p,q,r}; x, y)) \), 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

\[ P_{M_1}(S_{p,q,r}) = 16^a \times 24 pqr x^4 y^4 + 4(p + pr + qr)(9^a \times 2x^3 y^3 + 12^a \times 2x^3 y^4 - 16^a \times 3x^4 y^4) + 4(p + q + r)(9^a x^3 y^3 - 12^a \times 2x^3 y^4 + 16^a x^4 y^4). \]  

(20)

**Theorem 5.** Let \( S_{p,q,r} \) be a sodalite material, with \( p, q, r \geq 1 \), and \( P_{IR_1} \) be the M-polynomial of general inverse Randić index. Then, \( P_{IR_1}(S_{p,q,r}) \) is

\[ P_{IR_1}(S_{p,q,r}) = \frac{24}{16^a} pqr x^4 y^4 + 4(p + pr + qr)(\frac{2}{9} x^3 y^3 + \frac{2}{12} x^3 y^4 - \frac{3}{16} x^4 y^4) + 4(p + q + r)(\frac{1}{9} x^3 y^3 - \frac{2}{12} x^3 y^4 + \frac{1}{16} x^4 y^4). \]  

(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 \( P_{IR_1}(S_{p,q,r}) = (S_x^p S_y^q)(M(S_{p,q,r}; x, y)) \), 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

\[ P_{IR_1}(S_{p,q,r}) = \frac{24}{16^a} pqr x^4 y^4 + 4(p + pr + qr)(\frac{2}{9} x^3 y^3 + \frac{2}{12} x^3 y^4 - \frac{3}{16} x^4 y^4) + 4(p + q + r)(\frac{1}{9} x^3 y^3 - \frac{2}{12} x^3 y^4 + \frac{1}{16} x^4 y^4). \]  

(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,

\[ [D_x]_{(x,y)=(1,1)} = 96 pqr + 4(p + q + r), \]

\[ [D_y]_{(x,y)=(1,1)} = 96 pqr + 8(pq + pr + qr) - 4(p + q + r). \]  

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

\[ M_1(S_{pqr}) = 192pq + 8(pq + pr + qr), \]
\[ M_2(S_{pqr}) = 384pq - 24(pq + pr + qr) + 4(p + q + r). \] \hfill (25)

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

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

\[ M_1(S_{pqr}) = 192pq + 8(pq + pr + qr). \] \hfill (26)

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

\[ M_2(S_{pqr}) = 384pq - 24(pq + pr + qr) + 4(p + q + r). \] \hfill (27)

Theorem 7. Let $S_{pqr}$ be a sodalite material, with $p, q, r \geq 1$, and $^mM_3$ be the second modified Zagreb index. Then, $^mM_3(S_{pqr})$ is

\[ ^mM_3(S_{pqr}) = \frac{3}{2}pq + \frac{23}{36}(pq + pr + qr) + \frac{7}{36}(p + q + r). \] \hfill (28)

Proof. According to Definition 3, the formula for the M-polynomial of second modified Zagreb index for $S_{pqr}$ is defined as $^mM_3(S_{pqr}) = (S_x S_y)(M(S_{pqr}; x, y))$, by using the integral operators that are defined in Lemma 2 for $S_{pqr}$. After some algebraic simplifications, we will get the M-polynomial of second modified Zagreb index for $S_{pqr}$.

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

\[ (^mM_3)(S_{pqr}) = \frac{3}{2}pq + \frac{23}{36}(pq + pr + qr) + \frac{7}{36}(p + q + r). \] \hfill (29)

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

\[ R_a(S_{pqr}) = 16^a \times 24pq + 4(pq + pr + qr) \times (9^a \times 2 + 12^a \times 2 - 16^a \times 3) \]
\[ + 4(pq + pr + qr)(9^a - 12^a \times 2 + 16^a). \] \hfill (30)

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

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

\[ R_a(S_{pqr}) = 16^a \times 24pq + 4(pq + pr + qr) \times (9^a \times 2 + 12^a \times 2 - 16^a \times 3) \]
\[ + 4(pq + pr + qr)(9^a - 12^a \times 2 + 16^a). \] \hfill (31)

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

\[ ^aR_a(S_{pqr}) = \frac{24}{16^a} pq + 4(pq + pr + qr) \left( \frac{2}{9^a} + \frac{2}{12^a} - \frac{3}{16^a} \right) \]
\[ + 4(p + q + r) \left( \frac{1}{5^a} - \frac{2}{12^a} + \frac{1}{16^a} \right). \] \hfill (32)

Proof. According to Definition 4, the formula for the M-polynomial of general inverse Randić index for $S_{pqr}$ is defined as $^aR_a(S_{pqr}) = (S_x^a S_y^a)(M(S_{pqr}; x, y))$, by using the
Figure 2: General 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 4: Second Zagreb 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 6: General Randić M-polynomial for three-dimensional sodalite network $S_{4,4,4}$ and $\alpha = -(1/2)$.

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 $S_{pq,r}$. After some algebraic simplifications, we will get the M-polynomial of general inverse Randić index for $S_{pq,r}$.

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

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

(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 $S_{pq,r}$, 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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