Research Article

Topological Study of Zeolite Socony Mobil-5 via Degree-Based Topological Indices

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Received 2 March 2021; Accepted 26 May 2021; Published 24 June 2021

Academic Editor: Teodorico C. Ramalho

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Graph theory is a subdivision of discrete mathematics. In graph theory, a graph is made up of vertices connected through edges. Topological indices are numerical parameters or descriptors of graph. Topological index tells the symmetry of compound and helps us to compare those mathematical values, with boiling point, melting point, density, viscosity, hydrophobic surface area, polarity, etc., of that compound. In the present research paper, degree-based topological indices of Zeolite Socony Mobil-5 are calculated. Names of those topological indices are Randić index, first Zagreb index, general sum connectivity index, hyper-Zagreb index, geometric index, ABC index, etc.

1. Introduction

In graph theory, the term graph was suggested in eighteenth century by Leonhard Euler (1702–1782). He was a Swiss mathematician. He manipulated graphs to solve Konigsberg bridge problem [1–3]. Chemical graph theory is a topological division of mathematical chemistry that practices graph theory to model chemical structures mathematically. It studies chemistry and graph theory to view the detailed physical and chemical properties of compounds. A graph \( G = (V, E) \) is comprised through a set of vertices \( V \) and an edges set \( E \) [4].

Topological indices study the properties of graphs that remain constant/unchanged after continuous change in structure. Topological indices explain formation and symmetry of chemical compounds numerically and then help in advancement of QSAR (qualitative structure activity relationship) and QSPR (quantitative structure property relationship). Both QSAR and QSPR are used to build a relation among molecular structure and mathematical tools. These descriptors are helpful to correlate physio-chemical properties of compounds (enthalpy, boiling and melting point, strain energy, etc.) that is why these descriptors have a large number of applications in chemistry, biotechnology, nanotechnology, etc.

Topological indices are invariants of graph that is why topological indices are independent of pictorial representation of graph. In other words, it is a numerical value that describes the structure of chemical graph [5, 6]. Among the three types of topological indices, degree-based indices have great importance. The need to define these indices is to explain physical properties of every chemical structure with a number. Continuous change in shape does not affect the value of topological index. Topological indices are useful in the study of QSAR and QSPR because topological indices show the physical properties and convert the chemical structure into a numerical value.

Distance-based topological indices deal with distances of graph, degree-based topological indices use the concept of degree, and counting-based topological index depends upon counting the edges. Randić explained some characteristics of a topological index. Some of them are explained here.
A topological index should
(i) have architectural interpretation
(ii) be well-defined
(iii) be related with at least one physio-chemical property of compound
(iv) be uncomplicated
(v) display an appropriate size dependence
(vi) modify with modification in structure
(vii) locally defined
(viii) have related with other indices

Topological indices show translations of chemical compounds into distinctive structural descriptors as a numerical value that can be used by QSAR [7, 8]. Topological indices are awfully beneficial in describing the properties of given compound. Chemists can use these indices to correlate considerable range of characteristics. Medicine industry is developing new drug designs that are useful for humans, plants, and animals. Many graph theoretical techniques have been established for forecasting of medicinal, environmental, and physio-chemical properties of compounds. It is not astonishing to see such a great victory of graph theory and topological indices in analyzing biological and physical characteristics of chemical compounds.

1.1. ZSM. Zeolites (aluminosilicate) are tetrahedrally-linked structures based on silicate and aluminate tetrahedral. Structural chemistry deals with the framework of zeolites; it also works out on the arrangement of cations and other molecules in pore spaces. It belongs to a pentasil class of zeolite. It consists of silica (Si) and alumina (Al). It is named as ZSM-5 due to pore diameter of five angstrom; also, it has Si/Al ratio of five [9]. Size of the molecule depends on the type of structure. It is a crystalline powder. Geometry of pores can be connected in channels in one, two, or three dimensions.

1.1.1. Motivations. The structure of ZSM-5 has great importance in the field of chemistry, petroleum, and medicine industry. ZSM-5 is useful because of its stability, favorable selectivity, metal tolerance, and flexibility. It is also useful for the treatment of fertilizers. It helps to separate oxygen and nitrogen in the air. This unique structure is useful in petroleum industry as a catalyst. It is generally used in the conversion of methanol to gasoline as well as refining of oil. Through dehydration, it changes alcohol into petrol. Efficiency of LPG can also be increased through ZSM-5 catalyst. It keeps unusual hydrophobicity that is useful to separate hydrocarbons from polar compounds. Basic reason of calculation of topological indices is the industrial uses of ZSM-5 structure.

(1) First General Zagreb Index. This index was first presented by Li and Zhao. Its mathematical form is defined in [10–12] as follows:

\[ M_1(G) = \sum_{p\in V(G)} (d_p)^2. \]  

(2) First Zagreb Index. It is defined in [16, 17]:

\[ M_1(G) = \sum_{pq\in E(G)} (d_p + d_q). \]

(3) Second Zagreb Index. It is defined in [11, 16]:

\[ M_2(G) = \sum_{pq\in E(G)} (d_p \times d_q). \]

Multiple and polynomial Zagreb indices:
In 2012, new kinds of Zagreb indices were introduced by Ghorbani and Azimi, named as first and second multiple Zagreb indices represented as PM1 (G) and PM2 (G) [11, 15, 18]. The polynomials are used to find the Zagreb index. First and second Zagreb polynomial indices are written as M1 (G, j) and M2 (G, j).

(4) First and second multiple Zagreb indices:

\[ PM_1(G) = \prod_{pq\in E(G)} (d_p + d_q), \]

\[ PM_2(G) = \prod_{pq\in E(G)} (d_p \times d_q). \]

(5) First and second polynomial Zagreb indices:

\[ M_1(G, j) = \sum_{pq\in E(G)} j(d_p+d_q), \]

\[ M_2(G, j) = \sum_{pq\in E(G)} j(d_p\times d_q). \]

(6) Hyper-Zagreb Index. Modified Zagreb index is called hyper-Zagreb and that was introduced in 2013 by Shirdil, Rezapour, and Sayadi [19–21], mathematically written as

\[ HM(G) = \sum_{pq\in E(G)} (d_p + d_q)^2. \]

(7) Second modified Zagreb index:

\[ M_2(G) = \sum_{pq\in E(G)} \frac{1}{(d_p \times d_q)}. \]

(8) Reduced second Zagreb index. This index was proposed by Furtula and it is defined as

\[ RM_2(G) = \sum_{pq\in E(G)} (d_p - 1 \times d_q - 1). \]
(9) Atom Bond Connectivity Index. It was written in 1998 by Ernesto Estrada and Torres [15, 22–24]. It is used to model thermodynamic characteristics of organic compounds (especially alkanes). Mathematically,

\[
\text{ABC}(G) = \sum_{pq \in E(G)} \frac{d_p + d_q - 2}{d_p d_q}.
\]  

(10) Fourth Atom Bond Connectivity Index. In 2010, Ghorbani et al. introduced this index [13, 14]. It is written as ABC₄ index:

\[
\text{ABC}_4(G) = \sum_{pq \in E(G)} \sqrt{S_p + S_q - 2}.
\]  

(11) General Randić Connectivity Index. First degree-based TI was proposed in 1975 by Milan Randić. At that time, it was called as branching index [8, 17, 18] and used to measure the branching of hydrocarbons. In 1998, Eddrős and Bollobás wrote the general term of this index by changing the factor \((-1/2)\) with \(a\) \(\epsilon\) \(R\) [25]. It is defined as the total sum of weights \((d(p)d(q))^a\) of all the edges \(pq\), \(d(p)\) is the degree of \(p\), \(d(q)\) is the degree of \(q\), and \(a\) \(\epsilon\) \(R\).

\[
R_a(G) = \sum_{pq \in E(G)} (d_p d_q)^a.
\]  

(12) Randić index:

This index can also be called as first genuine degree-based topological index [15, 23]. Randić index is defined as

\[
R(G) = \sum_{pq \in E(G)} \frac{1}{\sqrt{d_p d_q}}.
\]  

(13) Reciprocal Randić Index. This index was first studied by Favaron, Mahéo, and Saclé [26]. The index is helpful in modeling of boiling points of hydrocarbons. It is defined as

\[
\text{RR}(G) = \sum_{pq \in E(G)} \sqrt{d_p d_q}.
\]  

(14) Reduced Reciprocal Randić Index. It is the analogue of reciprocal Randić index [26, 27]. It is defined as follows:

\[
\text{RRR}(G) = \sum_{pq \in E(G)} \sqrt{(d_p - 1)(d_q - 1)}.
\]  

(15) Geometric Arithmetic Index. GA index was proposed by Vukicević and Furtula [6, 14, 15]; it is stated as

\[
\text{GA}(G) = \sum_{pq \in E(G)} \frac{2}{d_p + d_q}.
\]  

(16) Fifth Geometric Arithmetic Index. In 2011, Grovac et al. introduced this index [7]. Mathematically, it is written as

\[
\text{GA}_5(G) = \sum_{pq \in E(G)} \frac{2\sqrt{S_p S_q}}{S_p + S_q}.
\]  

(17) Forgotten Index. This index was given by Gutman and Furtula in 2015 [16, 28, 29]. It is denoted by \(F\) (\(G\)) or \(F\) index:

\[
F(G) = \sum_{pq \in E(G)} (d_p^2 + d_q^2).
\]  

(18) General Sum Connectivity Index. The index was proposed by Zhou and Trinajstić [15, 23, 30]. Mathematically,

\[
\chi_a(G) = \sum_{pq \in E(G)} (d_p + d_q)^a,
\]  

where \(a\) \(\epsilon\) \(I\) \(R\).

(19) Symmetric Division Index. In 2010, Vukicević and Furtula proposed this useful index denoted by SD \((G)\) [28, 31, 32]:

\[
\text{SD}(G) = \sum_{pq \in E(G)} \frac{d_p^2 + d_q^2}{d_p d_q}.
\]  

(20) Harmonic Index. Siemion Fajtlowicz wrote a computer program that works for the automatic generation of conjectures in graph theory [11, 15]. He also examined the relationship between graph invariants; while doing this work, he found a vertex degree-based quantity. Later on, (in 2012) Zhang rediscovered that unknown quantity and named it as harmonic index. It is written as

\[
H(G) = \sum_{pq \in E(G)} \frac{2}{d_p + d_q}.
\]

2. Topological Indices of ZSM-5 Graphs

Topological indices remain constant for a given compound; they do not depend on the direction or position of graph. We can predict many physical properties of compounds such as solubility, soil sorption, boiling and melting properties, biodegradability, toxicity, vaporization, and thermodynamic properties.

2.1. Description of ZSM-5 Graph. The graph of ZSM-5 is given in Figure 1 and it is represented by \(G^*\). There are \(24pq + 4p\) vertices and \(36pq + 2p - 2q\) edges in \(G^*\).

**Theorem 1.** Let \(G^*\) be a graph of ZSM-5. Then, first general Zagreb index is
Theorem 1. \( G^* \) is a graph of ZSM-5. First Zagreb index is as follows:

\[
M_1(G) = \sum_{pq \in E(G)} (d_p + d_q),
\]

\[
M_1(G) = \sum_{pq \in E_1(G)} (d_p + d_q) + \sum_{pq \in E_2(G)} (d_p + d_q) + \sum_{pq \in E_3(G)} (d_p + d_q)
\]

\[= |E_1(G)|4 + |E_2(G)|5 + |E_3(G)|6 \]

\[= (4p)4 + (8p + 8q)5 + (36pq - 10p - 10q)6 \]

\[= 4p(4) + 8p(5) + 8q(5) + 36pq(6) - 10p(6) - 10q(6). \]

\[\square\]

Theorem 2. \( G^* \) is the graph of ZSM-5. First Zagreb index is as follows:

\[
M_1(G) = 4p2^a + (8p + 8q)2^a + (36pq - 10p - 10q)3^a.
\]

(23)

Proof. \( G^* \) is given in Figure 1. There are 24pq + 4p vertices, 8p + 4q of degree 2 vertices, and 24pq − 4p − 4q of degree 3 vertices.

Also, \( M_a(G^*) \) is defined as (1):

\[
M_a(G) = \sum_{p \in V(G)} (d_p)^a.
\]

(24)

We get \( M_a(G^*) \) by using the following formula:

\[
M_a(G^*) = 4p2^a + (8p + 8q)2^a + (36pq - 10n - 10p)3^a.
\]

(25)

Theorem 3. \( G^* \) is a graph of ZSM-5 and its 1st and 2nd polynomial Zagreb index is

(1) \( M_1(G^*, j) = (4p)j^4 + (8p + 8q)j^5 + (36pq - 10p - 10q)j^6; \)

(2) \( M_2(G^*, j) = (4p)j^4 + (8p + 8q)j^5 + (36pq - 10p - 10q)j^6. \)

\[
M_1(G) = -4p - 20q + 216pq.
\]

(26)

Proof. Assume \( G^* \) is a graph of ZSM-5. Then, \( E(G^*) \) is cleaved into 3 classes.

The 1st edges group \( E_1(G^*) \) contains 4p edges \( pq \), and \( d_p = d_q = 2 \).

The 2nd class \( E_2(G^*) \) has 8p + 8q edges \( pq \); here, \( d_p = 2, d_q = 3 \).

The 3rd arc division \( E_3(G^*) \) has 36pq − 10p − 10q arcs \( pq \); here, \( d_p = 3, d_q = 3 \).

It is easily understood that

\[
|E_1(G^*)| = e_2,2,
\]

\[
|E_2(G^*)| = e_2,3,
\]

\[
|E_3(G^*)| = e_3,3.
\]

We define \( M_1(G) \) in equation (29) as

\[
M_1(G) = \sum_{pq \in E(G)} (d_p + d_q),
\]

\[
M_1(G) = \sum_{pq \in E_1(G)} (d_p + d_q) + \sum_{pq \in E_2(G)} (d_p + d_q) + \sum_{pq \in E_3(G)} (d_p + d_q)
\]

\[= |E_1(G)|4 + |E_2(G)|5 + |E_3(G)|6 \]

\[= (4p)4 + (8p + 8q)5 + (36pq - 10p - 10q)6 \]

\[= 4p(4) + 8p(5) + 8q(5) + 36pq(6) - 10p(6) - 10q(6). \]

\[\square\]
\[ M_1(G, j) = \sum_{pq \in E(G)} j^{(d_p + d_q)}, \]  
(29)

\[ M_1(G^*, j) = \sum_{pq \in E_1(G^*)} j^{(d_p + d_q)} + \sum_{pq \in E_2(G^*)} j^{(d_p + d_q)} + \sum_{pq \in E_3(G^*)} j^{(d_p + d_q)} \]
= \sum_{pq \in E_1(G^*)} j^4 + \sum_{pq \in E_2(G^*)} j^5 + \sum_{pq \in E_3(G^*)} j^6 
= [E_1(G)] j^4 + [E_2(G)] j^5 + [E_3(G)] j^6 
= (4p) j^4 + (8p + 8q) j^5 + (36pq - 10p - 10q) j^6.
(30)

From (3), we have

\[ M_2(G, j) = \sum_{pq \in E(G)} j^{(d_p \times d_q)}, \]
\[ M_2(G^*, j) = \sum_{pq \in E_1(G^*)} j^{(d_p \times d_q)} + \sum_{pq \in E_2(G^*)} j^{(d_p \times d_q)} + \sum_{pq \in E_3(G^*)} j^{(d_p \times d_q)} \]
= \sum_{pq \in E_1(G^*)} j^4 + \sum_{pq \in E_2(G^*)} j^5 + \sum_{pq \in E_3(G^*)} j^6 
= [E_1(G^*)] j^4 + [E_2(G^*)] j^5 + [E_3(G^*)] j^6 
= (4p) j^4 + (8p + 8q) j^5 + (36pq - 10p - 10q) j^6,
(31)

which completes the proof.

\[ \square \]

**Theorem 4.** First and second multiple Zagreb index of \( G^* \) of ZSM-5 is given as

1. \( PM_1(G^*) = 4^{p^2} \times 5^{8p+8q} \times 6^{36pq-10p-10q} \).
2. \( PM_2(G^*) = 4^{p^2} \times 6^{8p+8q} \times 9^{36pq-10p-10q} \).

**Proof.** \( E(G^*) \) is classified into 3 edge classes based on the degree of end vertices. \( E_1(G^*) \) has 4p edges \( pq \), where \( d_p = d_q = 2 \). \( E_2(G^*) \) contains \( 8p + 8q \) edges \( pq \), where \( d_p = 2 \), \( d_q = 3 \). \( E_3(G^*) \) contains \( 36pq - 10p - 10q \) edges \( pq \), where \( d_p = 3 \), \( d_q = 3 \). Also consider \( |E_1(G^*)| = e_{2,2} \), \( |E_2(G^*)| = e_{2,3} \), and \( |E_3(G^*)| = e_{3,3} \). We define \( PM_1(G^*) \) as (4):

\[ PM_1(G^*) = \prod_{pq \in E(G^*)} (d_p + d_q), \]
\[ PM_1(G^*) = \prod_{pq \in E_1(G^*)} (d_p + d_q) \times \prod_{pq \in E_2(G^*)} (d_p + d_q) \times \prod_{pq \in E_3(G^*)} (d_p + d_q) \]
= \[4|E_1(G)| \times 5|E_2(G)| \times 6|E_3(G)| = 4^{p^2} \times 5^{8p+8q} \times 6^{36pq-10p-10q}. \]
(32)

Now, we define \( PM_2(G^*) \) as (5):

\[ PM_2(G) = \prod_{pq \in E(G)} (d_p \times d_q), \]
\[ PM_2(G^*) = \prod_{pq \in E_1(G^*)} (d_p \times d_q) \times \prod_{pq \in E_2(G^*)} (d_p \times d_q) \times \prod_{pq \in E_3(G^*)} (d_p \times d_q) \]
= \[4|E_1(G^*)| \times 6|E_2(G^*)| \times 9|E_3(G^*)| = 4^{p^2} \times 6^{8p+8q} \times 9^{36pq-10p-10q}. \]
(33)
which completes the proof.

\[HM(G^*) = 4p(16) + 8p(25) + 8q(25) + 36pq(36) - 10p(36) - 10q(36).\]  

(34)

**Theorem 5.** Then, hyper-Zagreb of \( G^* \) is written as follows:

\[|E_2(G^*)| = e_{2,3},\]

\[|E_3(G^*)| = e_{3,3},\]

(35)

Since, we have (8),

\[HM(G) = \sum_{pq \in E(G)} (d_p + d_q)^2,
\]

\[HM(G^*) = \sum_{pq \in E_1(G^*)} [d_p + d_q]^2 + \sum_{pq \in E_2(G^*)} [d_p + d_q]^2 + \sum_{pq \in E_3(G^*)} [d_p + d_q]^2\]

\[= 16|E_1(G^*)| + 25|E_2(G^*)| + 36|E_3(G^*)|\]

\[= 16(4p) + 25(8p + 8q) + 36(36pq - 10p - 10q)\]

\[= -96p - 160q + 1296pq,\]

which completes our proof.

\[\square\]

**Theorem 6.** \( G^* \) is the graph of ZSM-5. The second modified Zagreb index is given as

\[M_2(G^*) = \frac{1}{9}p + \frac{2}{9}q + 4pq.\]

(37)

**Proof.** Consider \( G^* \) to be a graph of ZSM-5. \( E(G^*) \) is divided into 3 sets based on the degree of end vertices. \( E_1(G^*) \) contains \( 4n \) edges \( pq \), where \( d_p = d_q = 2 \). \( E_2(G^*) \) holds \( 8p + 8q \) edges \( pq \), where \( d_p = 2 \), \( d_q = 3 \). \( E_3(G^*) \) holds \( 36pq - 10p - 10q \) edges \( pq \), where \( d_p = 3 \), \( d_q = 3 \). \( |E_1(G^*)| = e_{2,2}, \) \( |E_2(G^*)| = e_{2,3}, \) and \( |E_3(G^*)| = e_{3,3}. \)

We know the definition of \( M_2(G^*) \) as (9):

\[M_2(G) = \sum_{pq \in E(G)} \frac{1}{d_p \times d_q},\]

\[M_2(G^*) = |E_1(G^*)| \left(\frac{1}{4}\right) + |E_2(G^*)| \left(\frac{1}{6}\right) + |E_3(G^*)| \left(\frac{1}{9}\right)\]

\[= \frac{(4p)}{4} + \frac{(8p + 8q)}{6} + \frac{(36pq - 10p - 10q)}{9}\]

\[= \frac{11}{9}p + \frac{2}{9}q + 4pq.\]

(38)

\[\square\]

**Theorem 7.** Let \( G^* \) be the graph of ZSM-5. Then, reduced second Zagreb index is
Atombondconnectivityindexof
Theorem 8. Assume $G^*$ to be a graph of ZSM-5. $E\left( G^* \right)$ is divided into parts.

$E_1 \left(G^* \right)$ holds $4p$ edges $pq$, where $d_p = d_q = 2$.
$E_2 \left(G \right)$ has $8p + 8q$ lines $pq$, where $d_p = 2, d_q = 3$.
$E_3 \left(G^* \right)$ holds $36pq - 10p - 10q$ lines $pq$, where $d_p = 3, d_q = 3$. Also consider

$$RM_2 (G) = \sum_{pq \in E(G)} \left( d_p - 1 \times d_q - 1 \right),$$

$$RM_2 (G^*) = |E_1 (G^*)| (2 - 1)(2 - 1) + |E_2 (G^*)| (2 - 1)(3 - 1) + |E_3 (G^*)| (3 - 1)(3 - 1)$$

$$= (4p) + (8p + 8q)(2) \left( 36pq - 10p - 10q \right)(4)$$

$$= 4p + 8q(2) + 8p(2) + 36pq(4) - 10p(4) - 10q(4).$$

\[ \square \]

**Theorem 8.** Atom bond connectivity index of $G^*$ of ZSM-5 is as follows:

$$ABC(G^*) = 12p \left( \frac{1}{2\sqrt{2}} \right) + 8q \left( \frac{1}{2\sqrt{2}} \right) + 36pq \left( \frac{2}{3} \right)$$

$$- 10p \left( \frac{2}{3} \right) - 10q \left( \frac{2}{3} \right).$$

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}}$$

$$ABC(G^*) = |E_1 (G^*)| \left( \frac{1}{2\sqrt{2}} \right) + |E_2 (G^*)| \left( \frac{1}{2\sqrt{2}} \right) + |E_3 (G^*)| \left( \frac{2}{3} \right)$$

$$= (4p) \left( \frac{1}{2\sqrt{2}} \right) + (8p + 8q) \left( \frac{1}{2\sqrt{2}} \right) + \left( 36pq - 10p - 10q \right) \left( \frac{2}{3} \right)$$

$$= 4p \left( \frac{1}{2} \right) \sqrt{2} + \left( 8p \left( \frac{1}{2} \right) + 8q \left( \frac{1}{2} \right) \right) \sqrt{2} + 36pq \left( \frac{2}{3} \right)$$

$$- 10p \left( \frac{2}{3} \right) - 10q \left( \frac{2}{3} \right).$$

\[ \square \]

**Theorem 9.** ABC-4 index of ZSM-5 is as follows:

$$ABC_4 (G^*) = 4p \left( \frac{2}{5\sqrt{2}} \right) + \frac{4}{7\sqrt{14}} + 8p \left( \frac{1}{20\sqrt{110}} \right) - 4 + 4q \left( \frac{1}{42\sqrt{462}} \right)$$

$$+ 4p \left( \frac{1}{2} \right) + 2q \left( \frac{1}{3\sqrt{2}} \right) + 2p \left( \frac{1}{8\sqrt{14}} \right) + 12q \left( \frac{1}{12\sqrt{30}} \right)$$

$$+ 8p \left( \frac{1}{12\sqrt{30}} \right) + 36pq \left( \frac{4}{9} \right) - 24p \left( \frac{4}{9} \right) - 20q \left( \frac{4}{9} \right).$$
\textbf{Proof.} ZSM-5 has $36pq + 2p - 2q$ number of edges.

Consider an arc set relies on degree summation of neighbors of end vertices and $E(G^*)$ is divided into nine disjoint groups of edges, such as

$$E_i(G^*), \quad i = 5, 6, \ldots, 13;$$

here,

$$E(G^*) = \bigcup_{i=5}^{13} E_i(G^*).$$

$E_5(G^*)$ holds $4p$ number of edges $pq$, where $S_p = S_q = 5$, $E_6(G^*)$ has $4$ lines $pq$, where $S_p = 5$ and $S_q = 7$, $E_7(G^*)$ has $8p - 4$ edges $pq$, where $S_p = 5$ and $S_q = 8$, $E_8(G^*)$ has $4q + 4$ edges $pq$, where $S_p = 6$ and $S_q = 7$, $E_9(G^*)$ contains $4p - 4$ edges $pq$, where $S_p = 6$ and $S_q = 8$, $E_{10}(G^*)$ holds $2q + 4$ lines $pq$, where $S_p = 7$ and $S_q = 9$, $E_{11}(G^*)$ consists of $2p$ number of arcs $pq$, where $S_p = S_q = 8$, $E_{12}(G^*)$ has $12p + 8q - 16$ lines $pq$, where $S_p = 8$ and $S_q = 9$, and $E_{13}(G^*)$ contains $36pq - 24p - 20q + 12$ number of edges $pq$, where $S_p = S_q = 9$. The index is defined in equation (12):

$$\text{ABC}_4(G) = \sum_{pq \in E(G)} \sqrt{\frac{S_p + S_q - 2}{S_p S_q}},$$

$$\text{ABC}_4(G^*) = \sqrt[5]{\frac{5 + 5 - 2}{5 \times 5}} E_5(G^*) + \sqrt{\frac{5 + 7 - 2}{5 \times 7}} E_6(G^*) + \sqrt{\frac{5 + 8 - 2}{5 \times 8}} E_7(G^*)$$

$$+ \sqrt[6]{\frac{6 + 7 - 2}{6 \times 7}} E_8(G^*) + \sqrt{\frac{6 + 8 - 2}{6 \times 8}} E_9(G^*) + \sqrt{\frac{7 + 9 - 2}{7 \times 9}} E_{10}(G^*)$$

$$+ \sqrt[8]{\frac{8 + 8 - 2}{8 \times 8}} E_{11}(G^*) + \sqrt[9]{\frac{8 + 9 - 2}{8 \times 9}} E_{12}(G^*) + \sqrt[9]{\frac{9 + 9 - 2}{9 \times 9}} E_{13}(G^*)$$

$$= \sqrt{\frac{8}{25}} E_5(G^*) + \sqrt{\frac{10}{35}} E_6(G^*) + \sqrt{\frac{11}{40}} E_7(G^*) + \sqrt{\frac{11}{42}} E_8(G^*)$$

$$+ \sqrt{\frac{14}{63}} E_9(G^*) + \sqrt{\frac{14}{64}} E_{10}(G^*) + \sqrt{\frac{15}{72}} E_{11}(G^*) + \sqrt{\frac{16}{81}} E_{12}(G^*)$$

After putting the values of $E(G^*) = \bigcup_{i=5}^{13} E_i(G^*)$, we get

$$= \sqrt{\frac{8}{25}} (4p) + \sqrt{\frac{10}{35}} (4) + \sqrt{\frac{11}{40}} (8p - 4) + \sqrt{\frac{11}{42}} (4q + 4) + \sqrt{\frac{12}{48}} (4q - 4)$$

$$+ \sqrt{\frac{14}{63}} (2q + 4) + \sqrt{\frac{14}{64}} (2p) + \sqrt{\frac{15}{72}} (12p + 8q - 16) + \sqrt{\frac{16}{81}} (36pq - 24p - 20q + 12),$$

and after simplification,

$$= \frac{8}{5} \sqrt{2} p + \frac{4}{20} \sqrt{14} (8p - 4) + \frac{1}{42} \sqrt{462} (4q + 4) - \frac{62}{9} q + \frac{10}{3}$$

$$+ \frac{1}{3} \sqrt{2} (2q + 4) + \frac{1}{4} \sqrt{14} (2p) + \frac{1}{12} \sqrt{30} (12p + 8q - 16) + \sqrt{16} (36pq - 24p - 20q + 12).$$

\textbf{Theorem 10.} Let $G^*$ be the graph of ZSM-5. Fifth generation geometric arithmetic index is as follows:
Let $G^*$ be the graph of ZSM-5. Then, general Randic connectivity index is as follows:

$$GA_5(G) = 6p + \frac{2}{3\sqrt{35}} + \frac{4}{13} (8p - 4)\sqrt{10} + \frac{4}{13} q(2\sqrt{42}) + \frac{2297}{9282} + \frac{2}{q(8\sqrt{3})}$$

$$+ \frac{1}{q} (3\sqrt{7}) + \frac{12}{17} p(12\sqrt{2}) + \frac{8}{17} q(12\sqrt{2}) + 2pq(18) - \frac{4}{3} p(18)$$

(49)

**Proof.** ZSM-5 has $36pq + 2p - 2q$ number of edges.

Consider an arc set relies on degree summation of neighbors of end vertices and $E(G^*)$ is divided into nine disjoint groups of edges, such as

$$E_i(G^*), \quad i = 5, 6, \ldots, 13;$$

here,

$$E(G^*) = \bigcup_{i=5}^{13} E_i(G^*).$$

(50)

After putting the values $E(G^*) = \bigcup_{i=5}^{13} E_i(G^*)$, we get

$$= \frac{2\sqrt{25}}{10} (4p) + \frac{2\sqrt{35}}{12} (4) + \frac{2\sqrt{40}}{13} (8p - 4) + \frac{2\sqrt{42}}{13} (4q + 4) + \frac{2\sqrt{48}}{14} (4q - 4)$$

$$+ \frac{2\sqrt{63}}{16} (2q + 4) + \frac{2\sqrt{64}}{16} (2p) + \frac{2\sqrt{72}}{17} (12p + 8q - 16) + \frac{2\sqrt{81}}{18} (36pq - 24p - 20q + 12).$$

(52)

After simplification,

$$= -18p + \frac{2}{3\sqrt{35}} + \frac{4}{13} \sqrt{10} (8p - 4) + \frac{2}{13\sqrt{42}} (4q + 4) + \frac{4}{7\sqrt{3}} (4q - 4)$$

$$+ \frac{3}{8\sqrt{7}} (2q + 4) + \frac{12}{17} \sqrt{2} (12p + 8q - 16) + 36pq - 20q + 12.$$
\[ R_n(G^*) = 4p(4^*) + 8p(6^*) + 8q(6^*) + 36pq(9^*) - 10p(9^*) - 10q(9^*). \]  

(54)

**Proof.** The graph \( G^* \) of zeolite encounters 36pq + 2p - 2q edges and 24pq + 4p vertices.

The numeral of vertices of degree 2 are 8p + 4q and of degree 3 are 24pq - 4p - 4q. \( E \) of \( G^* \) are 36pq + 2p - 2q. \( E(G^*) \) is divided into three edge groups. \( E_1(G^*) \) has 4p edges \( pq \), where \( d_p = d_q = 2 \), \( E_2(G^*) \) contains 8p + 8q edges \( pq \), where \( d_p = 2 \) and \( d_q = 3 \), and \( E_3(G^*) \) supports 36pq - 10p - 10q arcs \( pq \), where \( d_p = d_q = 3 \).

By using definition of Randić index (13),

\[
R_n(G) = \sum_{pq \in E(G)} (d_p d_q)^{\alpha}. 
\]

(55)

Now, we have

After simplification, we get

\[ R_n(G^*) = \sum_{pq \in E_1(G^*)} (d_p d_q)^{\alpha} + \sum_{pq \in E_2(G^*)} (d_p d_q)^{\alpha} + \sum_{pq \in E_3(G^*)} (d_p d_q)^{\alpha} = 4|E_1(G^*)| + 6|E_2(G^*)| + 9|E_3(G^*)| = 4(4p) + 6(8p + 8q) + 9(36pq - 10p - 10q). \]

(56)

The numeral of vertices of degree 2 are 8p + 4q and of degree 3 are 24pq - 4p - 4q. \( E \) of \( G^* \) are 36pq + 2p - 2q. \( E(G^*) \) cleaves in three disunate edge groups:

\[ E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*). \]

(59)

\( E_1(G^*) \) has 4p arcs \( pq \), where \( d_p = d_q = 2 \), \( E_2(G^*) \) contains 8p + 8q edges \( pq \), where \( d_p = 2 \) and \( d_q = 3 \), and \( E_3(G^*) \) supports 36pq - 10p - 10q arcs \( pq \), where \( d_p = d_q = 3 \).

We define this index in equation (16):

\[ RRR(G^*) = \frac{4}{3}p + \frac{1}{6 \sqrt{6}}(8p + 8q) + 12pq - \frac{10}{3}q. \]

(58)

**Theorem 12.** Let \( G^* \) be the graph of ZSM-5. Then, the reciprocal Randić index is as follows:

\[
RRR(G^*) = \frac{4}{3}p + \frac{1}{6 \sqrt{6}}(8p + 8q) + 12pq - \frac{10}{3}q. \]

(58)

**Proof.** The graph \( G^* \) of zeolite encounters 36mm + 2n - 2m edges and 24pq + 4p vertices.

\[ RRR(G) = \sum_{pq \in E(G)} \sqrt{(d_p - 1)(d_q - 1)}, \]

\[ RRR(G^*) = \sum_{pq \in E_1(G^*)} \sqrt{(d_p - 1)(d_q - 1)} + \sum_{pq \in E_2(G^*)} \sqrt{(d_p - 1)(d_q - 1)} + \sum_{pq \in E_3(G^*)} \sqrt{(d_p - 1)(d_q - 1)} \]

(60)

\[ = 1|E_1(G^*)| + \sqrt{2}|E_2(G^*)| + 2|E_3(G^*)| = (4p) + \sqrt{2}(8p + 8q) + 2(36pq - 10p - 10q) = -16p + \sqrt{2}(8p + 8q) + 72pq - 20m. \]

(60)

The vertices of degree two are 8p + 4q and of degree three are 24pq - 4p - 4q. Cardinality of \( E \) of \( G^* \) is 36pq + 2p - 2q. The arc group \( E(G^*) \) cleaves in 3 disjoint arc groups that rely on the degrees of the end vertices, such as

\[ E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*). \]

(62)

\( E_1(G^*) \) has 4p lines \( pq \), where \( d_p = d_q = 2 \).

\( E_2(G^*) \) has 8p + 8q lines \( pq \), where \( d_p = 2 \) and \( d_q = 3 \).

**Theorem 13.** Consider \( G^* \) to be the graph of ZSM-5. Geometric arithmetic index is described as follows:

\[ GA(G^*) = \frac{2}{5 \sqrt{6}}(8p + 8q) + 36pq - 10p - 10q. \]

(61)

**Proof.** The graph \( G^* \) of zeolite encounters 36pq + 2p - 2q edges and 24pq + 4p vertices. The grouping of the vertices is given as follows:
Theorem 14. Forgotten index of graph $G^*$ of ZSM-5 is as follows:

$$F(G^*) = 4p(4) + 8p(13) + 8q(13) + 36pq(18) - 10p(18) - 10q(18).$$

(64)

Proof. The graph $G^*$ encounters $36pq + 2p - 2q$ edges and $24pq + 4p$ vertices.

The points of degree 2 are $8p + 4q$ and the points of degree 3 are $24pq - 4p - 4q$. The cardinality edge group $E$ of $G^*$ is $36pq + 2p - 2q$. $E(G^*)$ cleaves into three disjoint line groups that are as follows: $E_1(G^*)$ holds $4n$ arcs and $d_p = d_q = 2$. $E_2(G^*)$ supports $8n + 8m$ arcs $pq$, where $d_p = 2$ and $d_q = 3$, and $E_3(G^*)$ has $36m - 10n - 10m$ arcs $pq$, where $d_p = d_q = 3$.

By using the definition of forgotten index (19),

$$F(G) = \sum_{pq \in E(G)} (d_p^2 + d_q^2),$$

$$F(G^*) = \sum_{pq \in E_1(G^*)} (d_p^2 + d_q^2) + \sum_{pq \in E_2(G^*)} (d_p^2 + d_q^2) + \sum_{xy \in E_3(G^*)} (d_p^2 + d_q^2)$$

$$= 8|E_1(G^*)| + 13|E_2(G^*)| + 18|E_3(G^*)|$$

$$= 8(4p) + 13(8p + 8q) + 18(36pq - 10p - 10q)$$

$$= -44p - 76q + 648pq.$$  

(65)  

Theorem 15. Let $G^*$ be the graph of ZSM-5, then the general sum connectivity index is as follows:

$$X_n(G^*) = 4p(4^n) + 8p(5^n) + 8q(5^n) + 36pq(6^n) - 10p(6^n) - 10q(6^n).$$

(66)

Proof. The graph $G^*$ of zeolite encounters $36pq + 2p - 2q$ edges and $24pq + 4p$ vertices.

Vertices of degree two are $8n + 4m$ and of degree three are $24pq - 4p - 4q$. $E$ of $G^*$ are $36pq + 2p - 2q$. $E(G^*)$ cleaves into 3 disjoint edge groups. $E_1(G^*)$ holds $4p$ edges...
where $d_p = d_q = 2$, $E_2(G^*)$ holds $8p + 8q$ edges $pq$, where $d_p = 2$ and $d_q = 3$, $E_3(G^*)$ holds $36pq - 10p - 10q$ edges $pq$, where $d_p = d_q = 3$. From (20), we get the definition of general sum connectivity index:

$$X_a(G) = \sum_{pq \in E(G)} (d_p + d_q)^a,$$

$$X_a(G^*) = \sum_{pq \in E_4(G^*)} (d_p + d_q)^a + \sum_{pq \in E_5(G^*)} (d_p + d_q)^a + \sum_{x \neq y \in E_6(G^*)} (d_p + d_q)^a$$

$$= (4)^a|E_1(G^*)| + (5)^a|E_2(G^*)| + (6)^a|E_3(G^*)|$$

$$= (4)^a(4p) + (5)^a(8p + 8q) + (6)^a(36pq - 10q - 10p).$$

**Theorem 16.** $G^*$ is the graph of ZSM-5 and its symmetric division index is as follows:

$$SD(G^*) = \frac{16}{3}p - \frac{8}{3}q + 72pq. \quad (68)$$

**Proof.** $G^*$ of zeolite encounters $36pq + 2p - 2q$ edges and $24pq + 4p$ vertices.

The number of vertices of degree two are $8n + 4m$ and the number of vertices of degree three are $24pq - 4p - 4q$. $E$ of $G^*$ are $36pq + 2p - 2q$. $E(G^*)$ cleaves into three disjoint edge groups. $E_4(G^*)$ holds $4p$ edges $pq$, $E_5(G^*)$ holds $8p + 8q$ edges $pq$, and $E_6(G^*)$ holds $36pq - 10p - 10q$ edges $pq$, where $d_p = d_q = 3$.

From (21), we get

$$SD(G) = \sum_{pq \in E(G)} \frac{d_p^2 + d_q^2}{d_p \times d_q},$$

$$SD(G^*) = \sum_{pq \in E_4(G^*)} \frac{d_p^2 + d_q^2}{d_p \times d_q} + \sum_{pq \in E_5(G^*)} \frac{d_p^2 + d_q^2}{d_p \times d_q}$$

$$+ \sum_{pq \in E_6(G^*)} \frac{d_p^2 + d_q^2}{d_p \times d_q}$$

$$= (2)|E_1(G^*)| + \left(\frac{13}{5}\right)|E_2(G^*)| + (2)|E_3(G^*)|$$

$$= 2(4p) + \left(\frac{13}{5}\right)(8p + 8q) + 2(36pq - 10q - 10p). \quad (69)$$

After simple calculations,

$$= -12p + \frac{13}{5} + 72pq - 20q. \quad (70)$$

**Theorem 17.** $G^*$ is the graph of ZSM-5 and its harmonic index is as follows:

$$H(G) = \frac{4}{3}p + 8p(\frac{2}{5}) + 8q(\frac{2}{5}) + 12pq - \frac{10}{3}q. \quad (71)$$

$$H(G^*) = \sum_{pq \in E_4(G^*)} \frac{2}{d_p + d_q} + \sum_{pq \in E_5(G^*)} \frac{2}{d_p + d_q}$$

$$+ \sum_{pq \in E_6(G^*)} \frac{2}{d_p + d_q}$$

$$= \left(\frac{2}{4}\right)|E_1(G^*)| + \left(\frac{2}{5}\right)|E_2(G^*)| + \left(\frac{2}{6}\right)|E_3(G^*)|$$

$$= \left(\frac{1}{2}\right)(4p) + \left(\frac{2}{3}\right)(8p + 8q) + \left(\frac{1}{3}\right)(36pq - 10q - 10p)$$

$$= 2p + \left(\frac{1}{2}\right)(16p + 16q) + \left(\frac{2}{3}\right)(18pq - 5q - 5p)$$

$$= 37 \frac{10}{30}. \quad (72)$$

**3. Conclusion**

We correlate the uses of topological indices with chemical structure of ZSM-5. The main interest of the research is to present a concise introduction to some basic concepts about topological indices and their uses to find physicochemical properties of chemical structures. We conclude that physical properties of ZSM-5 can easily be calculated through topological indices. The consequences lay out noteworthy contribution in the field of graph theory and chemistry. This
research contains the results theoretically not experimentally.

**Data Availability**

No data were used in this study.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

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