Ve-degree and Ev-degree Based Topological Properties of Magnesium Oxide MgO (111) Structures

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Abstract

The topological index is a computational depiction of a molecular framework and estimates the physical property of a chemical compound. In the current research, we have developed clear indication of recently defined novel Ve-degrees and Ev-degrees dependent topographical index values of Magnesium Oxide MgO (111). For this by consider a unit cell of MgO (111) which is extended to its general structure. After that, we have calculated Ve-degrees and Ev-degrees of this general structure of MgO (111) then by employing well-known topological indices on these calculated Ve-degrees and Ev-degrees of the general structure, obtained numerical results. Different sorts of graphical constants have been explained and examined, presenting numerous practical applications in the area of nano-chemistry, computative webbing and indifferent scientific study fields. These computed results will help study the corporeal, chemical along with biological characteristics of the structure like melting, boiling and flickering point, moisture, forming heat, temperature, pressure and density etc.

Keywords: Ev-degree, Magnesium Oxide MgO, Ve-degree, Topological indices, Physical Properties.

1. Introduction

Several studies were carried out in the theory of chemical graphs which has led to the development and progress in the numerical transformation and duplication of chemical graphs. Chemical graph theory allows the scientists to develop a association among the graph theory and the chemical structure of chemical compounds. The workload in chemical graph theory has also been increased because of the speedy rise in the manufacture of present day medicines and chemical compounds by the chemical industry. Subsequently, it is important to examine entire chemical characteristics of these latest medicines and compounds to make appropriate use of them. Many studies have been carried out to understand the relation between chemical characteristics like melting point, freezing point, harmfulness, solubility, along with molecular structure (Katritzky et al., 2001; Katritzky et al., 1996). Quantitative structure-property relationships (QSPR) and quantitative structure activity relationships (QSAR) study the topology of chemical frameworks, relevant to medications, medical research, rational drug design and experiential science (Wiener, 1947). In the quantitative structure-property relationships field, after modelling different behaviours of chemical compounds were examined (Hosamni et al., 2017).

Topological indices foretells the physical characteristics. Bokhary et al., developed the QSPR among degree based indices and physical characteristics of breast cancer medicines to test the forecasting of indices (Bokhary et al., 2021). Linear regression model analysis showed that Randic index foretells the entropy, sum connectivity index value foretells the boiling point, forgotten index value foretells the molar mass and geometric arithmetic index value has particularly important correlation coefficient for melting point. Kirmani, S. A. K. et al., established the QSPR among degree based indices and phys-chemical characteristics of COVID medicines (Kirmani et al., 2021). They examined the forecasting of the
forgotten index for vaporization entropy, the second altered Zagreb index for ignition point, the Randic index for molar refractivity, the redefined third Zagreb index for polar contact area, and the rhythmic index for molar mass. Hosseini, H. et al. classifies the degree-based indices found on their forecasting ability. They elaborated the QSPR among indices and physical characteristics of the alkanes. They examined the high point association of Randic indices with heats of evaporation, atom-bond association index with boiling point, extended Zagreb indices with enthalpy of formation and geometric arithmetic indices along with enthalpy evaporation (Hosseini and Shafiei, 2016). For more relation of degree based indices see (Asok and Kureethara, 2018). Now, researchers are working to develop the relation among Ve-degree and Ev-degree dependent indices and physical characteristics (Ediz, 2017; Zhong et al., 2021; Rauf et al., 2022).

In determining the structural codes, theory of chemical graph performs a crucial part in this purpose. A molecule is viewed as a graph in the theory of chemical graphs, with its atoms acting like vertices and bonds (between atoms) being edges. For \( H = (V(H); E(H)) \) hence \( V = V(H) \) depicts the vertex set and \( E = E(H) \) depicts the edge set, representing the bonds among the atoms of the molecule, an improvised description of a graph \( H \) can be stated.

The topological index (TI) is the molecular graph’s numerical value used to describe the molecule. TI is invariant and serves as a useful mechanism for assigning a unique number to the molecule’s chemical structure, the unique number being independent of the graph’s labelling and drawing pattern (Naeem and Rauf, 2021). Topological indices (TI’s) are used for the creation of interactions between various compound properties. More precisely, TI compares the biological or chemical properties of the respective compound with the chemical structure. Wiener (Wiener, 1947) originally introduced the idea of a topological descriptor while working with paraffin and its indicant number is associated with the pivotal stage, vaporization temperature as well as density (Gutman et al., 1975; Nikolova and Jaworska, 2003). By using the edge, vertex degree idea, topography indices are utilized for comprehending as well as creating mathematical features of prototypes. Milan developed the Randić index in 1975 (Randic, 1975), and Bollobás et al. and Amic et al. generalized it later (Amic et al., 1998; Bollobas and Erdos, 1998). Gutman and Trinajstić gave the idea of the first Zagreb type index, the second Zagreb type index and the second-altered Zagreb type index (Gutman and Das, 2004; Das and Gutman, 2004). The Randic index is a variation of the Harmonic index. Zhong described the Harmonic index (Zhong, 2012), while Ediz et al. developed latest Harmonic indices (Ediz et al., 2017). However, the whole study was conducted using the traditional notion of degrees.

The numerical equations for a number of the Ev-degree and Ve-degree centered indices are presented in Table 1 describes about the morphological study of MgO (111) states that it is an ionic material retaining a typical rock salt structure (Ciston et al., 2008). MgO is also considered a stable inert ionic substance that acts as an amazing insulator with a bond width of 7.8 eV. MgO has a high melting point and has diverse applications in many commercial fields like electronics, optics, and cosmetics, etc (Zhu et al., 2006; Akbar et al., 2016). It acts as an effective substrate for many chemicals and is used as a catalyst also. MgO has a large surface area and has in toxic nature due to which it is used to remove dyes and also as an effective optical material (Baudin et al., 1997; Plass et al., 1998).

In this paper, we will discuss Magnesium Oxide (111) for \( s = 1,2,3,\ldots,s \). Figure 1 is the molecular structure of MgO(111). The crystal structure of Magnesium Oxide MgO(111) contains the \( 2(4s^2 + 4s + 1) \) vertices and \( 12s^2 + 8s + 1 \) edges.
Table 1: Ev-degrees and Ve-degree indices

| Ev-degree based topological indices | Notation | Numerical equation |
|-----------------------------------|----------|-------------------|
| Randić index                      | $R^{ev}$ | $\sum_{e \in E} N_{ev}(e)^{-\frac{1}{2}}$ |
| Zagreb index                      | $M^{ev}$ | $\sum_{e \in E} N_{ev}(e)^{2}$ |
| Ve-degree based topological indices | Notation | Mathematical Formula |
| First Zagreb $\beta$-index        | $M_{1}^{\beta ve}$ | $\sum_{uv \in E} [N_{ve}(u) + N_{ve}(v)]$ |
| Second Zagreb $\beta$-index       | $M_{2}^{\beta ve}$ | $\sum_{uv \in E} [N_{ve}(u) \times N_{ve}(v)]$ |
| Harmonic index                    | $H^{ve}$ | $\sum_{uv \in E} \frac{2}{N_{ve}(u) + N_{ve}(v)}$ |
| Sum Connectivity index            | $\chi^{ve}$ | $\sum_{uv \in E} [N_{ve}(u) + N_{ve}(v)]^{-\frac{1}{2}}$ |
| Geometric Arithmetic index        | $G^A^{ve}$ | $\sum_{uv \in E} \frac{2\sqrt{N_{ve}(u) \times N_{ve}(v)}}{(N_{ve}(u) + N_{ve}(v))}$ |
| Atom Bond Connectivity index      | $ABC^{ve}$ | $\sum_{uv \in E} \frac{N_{ve}(u) + N_{ve}(v) - 2}{(N_{ve}(u) \times N_{ve}(v))}$ |
| Randić index                      | $R^{ve}$ | $\sum_{uv \in E} [N_{ve}(u) \times N_{ve}(v)]^{-\frac{1}{2}}$ |
| First Zagreb $\alpha$-index       | $M_{1}^{ave}$ | $\sum_{v \in V(H)} N_{ve}(v)^{2}$ |

For $s=1$

For $s=2$

For $s=3$

Figure 1: Structure of Magnesium Oxide (111) for $s = 1$, $s = 2$ and $s = 3$

2. Methodology

We have considered a unit cell of MgO (111) then it is extended to its general structure. We calculated Ve-degrees and Ev-degrees of the general structure of MgO (111) then by employing well-known topological indices on these calculated Ve-degrees and Ev-degrees of the general structure, to obtain
required results. To compute the Ev-degree, Ve-degree, along with Ve-degree of the end points of every edge, numerical results and their graphical representation the MATLAB (MATLAB, 2019) has been used.

3. Results and Discussion

**Theorem 1** Let $H$ be a structure of Magnesium Oxide (111), then

(a) $M^{ev}(H) = 432s^2 + 112s + 18$.

(b) $R^{ev}(H) = \frac{12}{\sqrt{6}}s^2 + \left(\frac{16}{\sqrt{6}} - \frac{8}{\sqrt{6}}\right)s + \left(\frac{2}{\sqrt{3}} + 2 - \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right)$.

**Proof 1** To calculate the Ev-degree Zagreb and ev degree Randić index of MgO(111), it is mandatory to calculate the Ev degree of the edges in every divided set $E_{(i,j)}$. This computation is given in Table 2. At present utilising the details given in Table 2 and the definition of Ev-degree Zagreb and Randić index, we obtain.

From Table 2, (a) The ev-degree Zagreb index

$$M^{ev}(H) = \sum_{e \in E(H)} k_{ev}(e)^2,$$

$$M^{ev}(H) = (3)^2|E_{(1,2)}| + (4)^2|E_{(2,2)}| + (5)^2|E_{(2,3)}| + (6)^2|E_{(3,3)}|$$

$$= 2 \times 9 + 4 \times 16 + (16s - 4) \times 25 + (4s(3s - 2) + 1) \times 36$$

$$= 432s^2 + 112s + 18.$$

(b) The ev-degree Randić index

$$R^{ev}(H) = \sum_{e \in E(H)} k_{ev}(e)^{-\frac{1}{2}},$$

$$R^{ev}(H) = (3)^{-\frac{1}{2}}|E_{(1,2)}| + (4)^{-\frac{1}{2}}|E_{(2,2)}| + (5)^{-\frac{1}{2}}|E_{(2,3)}| + (6)^{-\frac{1}{2}}|E_{(3,3)}|$$

$$= 2 \times (3^{-\frac{1}{2}} + 4 \times (4)^{-\frac{1}{2}} + 4(4s - 1) \times (5)^{-\frac{1}{2}} + (12s^2 - 8s + 1) \times (6)^{-\frac{1}{2}}$$

$$= \frac{12}{\sqrt{6}}s^2 + \left(\frac{16}{\sqrt{6}} - \frac{8}{\sqrt{6}}\right)s + \left(\frac{2}{\sqrt{3}} + 2 - \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right).$$

| $(\mathbf{S}(u), \mathbf{S}(v))$ | $k_{ev}(e)$ | Frequency |
|-----------------------------|-------------|-----------|
| $E_{(1,2)}$                 | 3           | 2         |
| $E_{(2,2)}$                 | 4           | 4         |
| $E_{(2,3)}$                 | 5           | 4(4s - 1) |
| $E_{(3,3)}$                 | 6           | 4s(3s - 2) + 1 |

Table 2: The edges ev-degree of Magnesium Oxide MgO(111)

Numerical computation of the Ev-degree dependent indices shows a rising pattern as we raise the value of $s$. Topological indices predict physical properties. Zhong, Jian-Feng, et al. established the quantitative structure-property relationship (QSPR) among physical characteristics (Docking Score, Attaching Affinity, Molar mass and Topographical Polar exterior) and indices (Ve- and Ev-degree based) (Zhong et al., 2021). Zhong, Jian-Feng, et al. tested that in Ev-degree dependent indices, the first Ev-degree Zagreb index ($M^{ev}$) forecasts the molar mass greater than Ev-degree Randić index ($R^{ev}$). So, the given conclusion of Ev-degree dependent indices are beneficial to calculate the physical characteristics of MgO(111).

**Theorem 2** suppose $H$ be a complex arrangement of MgO(111), then vertices ve-degrees first Zagreb $\alpha$-index is designated

$$M^{ev}_1(H) = 648s^2 + 32s - 20.$$
Proof 2 via structure of MgO(111), we partitioned the vertices into six separations on the ground of degrees $V_1$, $V_2$, $V_3$, $V_4$, $V_5$ and $V_6$ respectively, where $|V(H)| = 2(4s^2 + 4s + 1)$.

| Table 3: The vertices ve-degrees of MgO(111) |
|--------------------------------------------|
| $\kappa(u)$ | $\kappa_{ve}(u)$ | Frequency |
| 1 | 2 | 2 |
| 2 | 5 | 4 |
| 2 | 6 | 4(2s − 1) |
| 3 | 5 | 2 |
| 3 | 7 | 4(2s − 1) |
| 3 | 9 | 2(4s^2 − 4s + 1) |

By using the above Table 3, we have the first ve-degree based Zagreb $\alpha$-index.

$$M_1^{ave}(H) = \sum_{v \in V(H)} \kappa_{ve}(v)^2$$

$$M_1^{ave}(H) = 2 \times (2)^2 + 4 \times (5)^2 + 4(2s − 1) \times (6)^2 + 2 \times (5)^2 + 4(2s − 1) \times (7)^2$$

$$+ 2(4s^2 − 4s + 1) \times (9)^2$$

$$= 648s^2 + 32s − 20.$$ Numerical Computation of the Ve-degree based first Zagreb alpha index ($M_1^{ave}$) indicates a rising pattern as we rise the rate of $s$. The topological index is a predictor of physical property. Ediz established QSPR among physical characteristics (Acentric factor, heat of vaporization (HVAP), Standard enthalpy of evaporation (DHVAP), and Entropy.) as well as indices (Ediz, 2017). Ediz developed analysis only for Ve and Ev-degree dependent Zagreb and Randić kind of indices. Ediz tested in such a way that $M_1^{ave}$foretells the physical characteristics Acentric Value. Zhong, Jian-Feng, et al. established the QSPR among physical characteristics (Binding Affinity, Docking rate, Molecular mass, and Topographical Polar area) as well as indices (Ve- and Ev-degree based) (Zhong et al., 2021). Zhong, Jian-Feng, et al. analyze that Ev-degree Randić index ($R_{ve}$) is weaker predictor of molecular mass than $M_1^{ave}$. So, the given conclusion of Ve-degree based index is useful in measuring the physical characteristics of Magnesium Oxide MgO(111).

Theorem 3 Let $H$ be a structure of Magnesium Oxide MgO(111), then end vertices ve-degrees based indices of each edge,

(a) $M_1^{\beta ve}(H) = 216s^2 + 48s − 2$.
(b) $M_2^{\beta ve}(H) = 972s^2 − 120s − 11$.
(c) $ABC^{ve}(H) = 4\sqrt{7}s^2 + \left(\frac{16\sqrt{13}}{\sqrt{42}} + \frac{32}{3\sqrt{7}} - \frac{16\sqrt{2}}{3}\right)s + \left(\frac{2\sqrt{2}}{\sqrt{5}} + \frac{4\sqrt{2}}{5} + \frac{4\sqrt{11}}{\sqrt{30}} + \frac{8\sqrt{3}}{\sqrt{35}} - \frac{12\sqrt{13}}{\sqrt{42}} - \frac{16}{3\sqrt{7}} + \frac{5\sqrt{2}}{3}\right)$.
(d) $GA^{ve}(H) = 12s^2 + \left(\frac{32\sqrt{42}}{13} + 3\sqrt{7} - 16\right)s + \left(\frac{\sqrt{13}}{2} + \frac{8\sqrt{30}}{11} + \frac{2\sqrt{35}}{3} - \frac{24\sqrt{42}}{13} - \frac{3\sqrt{7}}{2} + 7\right)$.
(e) $H^{ve}(H) = \frac{4}{3}s^2 + \left(\frac{32}{13} - \frac{16}{9} + 1\right)s + \left(\frac{2}{5} + \frac{8}{11} - \frac{24}{13} + \frac{2}{3} + \frac{5}{6}\right)$.
(f) $\chi^{ve}(H) = \frac{4}{3}s^2 + \left(\frac{16}{\sqrt{42}} - \frac{16}{\sqrt{18}} + 2\right)s + \left(\frac{1}{\sqrt{10}} + \frac{2}{\sqrt{11}} + \frac{4}{\sqrt{12}} + \frac{4}{\sqrt{18}} - \frac{12}{\sqrt{13}} - 1\right)$.
(g) $R^{ve}(H) = \frac{4}{3}s^2 + \left(\frac{16}{\sqrt{42}} + \frac{8}{3\sqrt{7}} - \frac{16}{9}\right)s + \left(\frac{2}{\sqrt{15}} + \frac{2}{5} - \frac{4}{\sqrt{30}} + \frac{4}{\sqrt{35}} - \frac{12}{\sqrt{42}} - \frac{4}{3\sqrt{7}} + \frac{5}{9}\right)$.

Proof 3 To calculate the Ve degree indices, we must first determine the point separation of $E(H)$.
dependent on the Ve degree of all edge’s peak vertices. This separation is described in detail in Table 4. Currently, utilizing the data given in Table 4 as well as the interpretation of Ve degree indices, we get

| Table 4: Edge partition of Magnesium Oxide MgO(111) |
|---|---|---|
| Edge | (\(\kappa_{ve}(u), \kappa_{ve}(v)\)) | Frequency |
|---|---|---|
| \(E_1\) | (3, 5) | 2 |
| \(E_2\) | (5, 5) | 2 |
| \(E_3\) | (6, 5) | 4 |
| \(E_4\) | (5, 7) | 4 |
| \(E_5\) | (6, 7) | 4(4s - 3) |
| \(E_6\) | (7, 9) | 4(2s - 1) |
| \(E_7\) | (9, 9) | 12s^2 - 16s + 5 |

By using the Table 4,

(a) The first Zagreb \(\beta\)-index

\[
M_1^{\beta ve}(H) = \sum_{uv \in E(H)} (\kappa_{ve}(u) + \kappa_{ve}(v))
\]

\[
M_1^{\beta ve}(H) = (8)|E_1| + (10)|E_2| + (11)|E_3| + (12)|E_4| + (13)|E_5| + (16)|E_6| + (18)|E_7|
\]

\[
= 2 \times 8 + 2 \times 10 + 4 \times 11 + 4 \times 12 + 4(4s - 3) \times 13 + 4(2s - 1) \times 16
\]

\[
+ (12s^2 - 16s + 5) \times 18
\]

\[
= 216s^2 + 48s - 2.
\]

(b) The second Zagreb \(\beta\)-index

\[
M_2^{\beta ve}(H) = \sum_{uv \in E(H)} (\kappa_{ve}(u) \times \kappa_{ve}(v))
\]

\[
M_2^{\beta ve}(H) = (15)|E_1|^2 + (25)|E_2|^2 + (30)|E_3|^2 + (35)|E_4|^2 + (42)|E_5|^2 + (63)|E_6|^2 + (81)|E_7|^2
\]

\[
= 2 \times 15 + 2 \times 25 + 4 \times 30 + 4 \times 35 + 4(4s - 3) \times 42 + 4(2s - 10) \times 63
\]

\[
+ (12s^2 - 16s + 5) \times 81
\]

\[
= 972s^2 - 120s - 11.
\]

(c) The Atom-bond connectivity index

\[
ABC^{ve}(H) = \sum_{uv \in E(H)} \sqrt{\frac{\kappa_{ve}(u) + \kappa_{ve}(v) - 2}{\kappa_{ve}(u) \times \kappa_{ve}(v)}}
\]

\[
ABC^{ve}(H) = \left(\frac{2}{15}\right)|E_1|^2 + \left(\frac{8}{25}\right)|E_2|^2 + \left(\frac{11}{30}\right)|E_3|^2 + \left(\frac{12}{35}\right)|E_4|^2 + \left(\frac{13}{42}\right)|E_5|^2
\]

\[
+ \left(\frac{16}{63}\right)|E_6|^2 + \left(\frac{18}{81}\right)|E_7|^2
\]

\[
= 2 \times \frac{2}{15} + 2 \times \frac{8}{25} + 4 \times \frac{11}{30} + 4 \times \frac{12}{35} + 4(4s - 3) \times \frac{13}{42}
\]

\[
+ 4(2s - 1) \times \frac{16}{63} + (12s^2 - 16s + 5) \times \frac{18}{81}
\]

\[
= 4\sqrt{2}s^2 + \left(\frac{16\sqrt{3}}{\sqrt{42}} + \frac{32}{3\sqrt{7}} - \frac{16\sqrt{3}}{\sqrt{42}}\right)s + \left(\frac{2\sqrt{7}}{\sqrt{5}} + \frac{4}{\sqrt{5}} + \frac{4\sqrt{17}}{\sqrt{30}} + \frac{8\sqrt{3}}{\sqrt{35}}\right)
\]

\[
- \frac{12\sqrt{17}}{\sqrt{42}} - \frac{16}{\sqrt{3\sqrt{7}}} + \frac{5\sqrt{2}}{3}.
\]

(d) The Geometric-arithmetic index
\[
\text{GA}^{ve}(H) = \sum_{uv \in E(H)} \frac{2 \sqrt{K_{ve}(u) \times K_{ve}(v)}}{(K_{ve}(u) + K_{ve}(v))}
\]
\[
\text{GA}^{ve}(H) = \left(\frac{2\sqrt{15}}{8}\right)|E^1_1| + \left(\frac{2\sqrt{25}}{10}\right)|E^2_2| + \left(\frac{2\sqrt{30}}{11}\right)|E^3_3| + \left(\frac{2\sqrt{35}}{12}\right)|E^4_4| + \left(\frac{2\sqrt{42}}{13}\right)|E^5_5|
\]
\[
+\left(\frac{2\sqrt{55}}{16}\right)|E^6_6| + \left(\frac{2\sqrt{55}}{18}\right)|E^7_7|
\]
\[
= 2 \times \frac{2\sqrt{15}}{8} + 2 \times \frac{2\sqrt{25}}{10} + 4 \times \frac{2\sqrt{30}}{11} + 4 \times \frac{2\sqrt{35}}{12} + 4(4s - 3) \times \frac{2\sqrt{42}}{13}
\]
\[
+4(2s - 1) \times \frac{2\sqrt{63}}{16} + (12s^2 - 16s + 5) \times \frac{2\sqrt{51}}{18}
\]
\[
= 12s^2 + \left(\frac{32\sqrt{42}}{13} + 3\sqrt{7} - 16\right)s + \left(\frac{\sqrt{15}}{2} + \frac{8\sqrt{30}}{11} + \frac{2\sqrt{35}}{3} + 8\sqrt{42} - \frac{3\sqrt{7}}{2} + 7\right).
\]

(e) The Harmonic index
\[
\text{H}^{ve}(H) = \sum_{uv \in E(H)} \frac{2}{K_{ve}(u) + K_{ve}(v)}
\]
\[
\text{H}^{ve}(H) = \left(\frac{2}{9}\right)|E^1_1| + \left(\frac{2}{10}\right)|E^2_2| + \left(\frac{2}{11}\right)|E^3_3| + \left(\frac{2}{12}\right)|E^4_4| + \left(\frac{2}{13}\right)|E^5_5| + \left(\frac{2}{14}\right)|E^6_6| + \left(\frac{2}{15}\right)|E^7_7|
\]
\[
= 2 \times \frac{2}{9} + 2 \times \frac{2}{10} + 4 \times \frac{2}{11} + 4 \times \frac{2}{12} + 4(4s - 3) \times \frac{2}{13} + 4(2s - 1) \times \frac{2}{15}
\]
\[
+(12s^2 - 16s + 5) \times \frac{2}{18}
\]
\[
= \frac{4}{3}s^2 + \left(\frac{32}{13} - \frac{16}{9} + 1\right)s + \left(\frac{2}{5} + \frac{8}{11} - \frac{4}{3} + \frac{2}{3} + \frac{5}{6}\right).
\]

(f) The Sum-connectivity index
\[
\chi^{ve}(H) = \sum_{uv \in E(H)} (K_{ve}(u) + K_{ve}(v))^{-\frac{1}{2}}
\]
\[
\chi^{ve}(H) = (8)^{-\frac{1}{2}}|E^1_1| + (10)^{-\frac{1}{2}}|E^2_2| + (11)^{-\frac{1}{2}}|E^3_3| + (12)^{-\frac{1}{2}}|E^4_4| + (13)^{-\frac{1}{2}}|E^5_5| + (16)^{-\frac{1}{2}}|E^6_6|
\]
\[
+\left(18\right)^{-\frac{1}{2}}|E^7_7|
\]
\[
= \frac{2}{\sqrt{8}} + \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{4}{\sqrt{12}} + \frac{4(4s - 3)}{\sqrt{13}} + \frac{4(2s - 1)}{\sqrt{14}} + \frac{12s^2 - 16s + 5}{\sqrt{15}}
\]
\[
= \frac{4}{\sqrt{2}}s^2 + \left(\frac{16}{\sqrt{15}} - \frac{16}{\sqrt{19}} + 2\right)s + \left(\frac{1}{\sqrt{2}} + \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{4}{\sqrt{12}} + \frac{4}{\sqrt{15}} - \frac{12}{\sqrt{15}}\right)
\]

(g) The Randić index
\[
\text{R}^{ve}(H) = \sum_{uv \in E(H)} (K_{ve}(u) \times K_{ve}(v))^{-\frac{1}{2}}
\]
\[
\text{R}^{ve}(H) = (15)^{-\frac{1}{2}}|E^1_1| + (25)^{-\frac{1}{2}}|E^2_2| + (30)^{-\frac{1}{2}}|E^3_3| + (35)^{-\frac{1}{2}}|E^4_4| + (42)^{-\frac{1}{2}}|E^5_5| + (63)^{-\frac{1}{2}}|E^6_6|
\]
\[
+\left(81\right)^{-\frac{1}{2}}|E^7_7|
\]
\[
= 2 \times (15)^{-\frac{1}{2}} + 2 \times (25)^{-\frac{1}{2}} + 4 \times (30)^{-\frac{1}{2}} + 4 \times (35)^{-\frac{1}{2}} + 4(4s - 3) \times (42)^{-\frac{1}{2}}
\]
\[
+4(2s - 1) \times (63)^{-\frac{1}{2}} + (12s^2 - 16s + 5) \times (81)^{-\frac{1}{2}}
\]
\[
= \frac{4}{3}s^2 + \left(\frac{16}{\sqrt{42}} + \frac{8}{3\sqrt{7}} - \frac{16}{\sqrt{9}}\right)s + \left(\frac{2}{\sqrt{15}} + \frac{2}{5} - \frac{4}{\sqrt{30}} + \frac{4}{\sqrt{35}} - \frac{12}{\sqrt{42}} - \frac{4}{\sqrt{5}} + \frac{5}{9}\right).
\]

Numerical Computation of the index values relying upon Ve-degree of terminal vertices of every edge exhibits a steadily rising trend when we raise the rate of s. Topological indices predict physical properties. Ediz examines that QSPR between physical properties and indices. Ediz examines that Ve-degree of point vertices dependent second Zagreb beta index value foretells the enthalpy and the Randić index value forecasts the Enthalpy of evaporation and Standard enthalpy of vaporization, correspondingly (Ediz, 2017). Zhong, Jian-Feng, et al. examined the QSPR among physical characteristics as well as indices (Ve- and Ev-degree based). Zhong, Jian-Feng, et al. examined that the first Ve-degree Zagreb beta index value (\(M^1_{ve}\)) foretells the molecular mass and Topographical Polar area greater than other Ve-degree of
peak vertices dependent index values. In general, $M_1^{\text{Rve}}$ is better foreteller of the molecular mass and Topographical Polar surface area in all Ve- and Ev-degree dependent index values (Zhong et al., 2021). So, the above results of Ve-degree of point vertices of every edge-based index values are useful for computing the physical characteristics of Magnesium Oxide MgO (111).

TIs are critical tools for analyzing chemical compounds because they take into account the fundamental topology of structures. Several well-known established topological indices; the indices of the Zagreb type were discovered to arise while computing the total $\pi$ –electron strength of molecules. The Randić index value is often applied to measure the chemical resemblance of the compounds and to determine the boiling point as well as Kovats constants of molecules due to its rising values indicating that the total $\pi$ –electron strength is rising and The ABC index value gives an excellent association for determining the stretching energy of linear and branched chemical structures, as well as for their stability.

From Table 5 and Table 6 we may see that, when we rise the values of (s), the Zagreb type’s index values also increase showing that for higher values of $s$. We may observe that with the rise in the value of $s$, the Randić index for Magnesium Oxide MgO(111) also increases. Similarly, The GA index for the Magnesium Oxide MgO(111) increases with the increase in $s$. For the Magnesium Oxide MgO(111) structure the ABC index also rise with the rise in valueof $s$. This represents that the stretching energy along with the stability of these linear and branched chemical structures are higher for larger values of $s$.

Overall we may say that when we increase the values of $s$, the considered topological descriptors also increase for Magnesium Oxide MgO(111) structure.

**Table 5: Numerical results of indices for Magnesium Oxide MgO(111)**

| $s$  | $M^{\text{ve}}$ | $M_1^{\text{Rve}}$ | $M_1^{\text{Bve}}$ | $M_2^{\text{Bve}}$ | $R_1^{\text{Bve}}$ |
|-----|----------------|--------------------|--------------------|--------------------|----------------|
| [1] | 544            | 660                | 262                | 841                | 3.5551         |
| [2] | 1952           | 2636               | 958                | 3637               | 9.2541         |
| [3] | 4224           | 5908               | 2086               | 8377               | 17.6197        |
| [4] | 7360           | 10476              | 3646               | 15061              | 28.6520        |
| [5] | 11360          | 16340              | 5638               | 23689              | 42.3510        |
| [6] | 16224          | 23500              | 8062               | 34261              | 58.7167        |
| [7] | 21952          | 31956              | 10918              | 46777              | 77.7490        |
| [8] | 28544          | 41708              | 14206              | 61237              | 99.4480        |
| [9] | 36000          | 52756              | 17926              | 77641              | 123.8136       |
| [10]| 44320          | 65100              | 22078              | 95989              | 150.8459       |

**Table 6: Numerical results of indices for Magnesium Oxide MgO(111)**

| $s$  | $R^{\text{ve}}$ | ABC$^{\text{ve}}$ | GA$^{\text{ve}}$ | $H^{\text{ve}}$ | $\chi^{\text{ve}}$ |
|-----|----------------|------------------|----------------|----------------|----------------|
| [1] | 17.49768       | 11.8713172       | 35.42962598    | 3.7982129      | 9.81664705    |
| [2] | 57.387111      | 34.234465        | 84.70021324    | 9.4819736      | 24.7395299    |
| [3] | 121.276542     | 67.9094599       | 157.970801     | 17.832401      | 45.3192672    |
| [4] | 209.165973     | 122.898167       | 255.241388     | 28.849495      | 71.555859     |
| [5] | 321.055404     | 11.873172        | 376.511998     | 42.533256      | 103.449304    |
| [6] | 456.944836     | 34.234462        | 521.782562     | 58.883683      | 140.999604    |
| [7] | 616.834267     | 67.9094599       | 691.0531498    | 77.90078       | 184.206759    |
| [8] | 800.723698     | 11.898167        | 884.323737     | 99.5844577     | 233.0707669   |
| [9] | 1008.61313     | 507.547328       | 101.594324     | 123.934965     | 287.5916296   |
| [10]| 1240.50266     | 620.418285       | 1342.8649114   | 150.95206      | 347.769347    |
4. Conclusion

Graph constants are determined by some famous topological index values which are useful for matching and predicting the characteristics of chemical compounds in QSPRs and the QSARs. The topological index (TI) predicts the physical properties. In this paper, we have calculated the Ev-degree & Ve-degree dependent topographical index values for the molecular framework of Magnesium Oxide (111) for a better perception of medicational, physical, chemical and biotic characteristics. We have investigated that with an increase in the values of \( s \), the considered topological descriptors also increase for MgO(111) structure. Different sorts of graphical constants have been elaborated and examined, presenting numerous useful jobs in the discipline of nano-chemistry, medical, computational frameworks and in numerous areas of scientific research. These investigated numerical results will be helpful for chemists, pharmacists and researchers for studying the pharmaceutical, physical, biotic and chemical characteristics of the structure.

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