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 trasnformation 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 experiental 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 physic-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. Hossenni, 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.

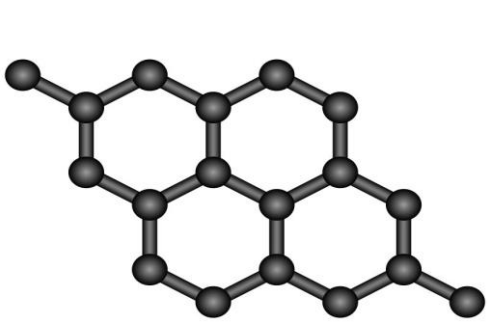
The topological index (TI) is the molecular graph's numerical value used to describe the molecule. TI is invariant and serves as a useful mechanism for assigning a unique number to the molecule's chemical structure, the unique number being independent of the graph's labelling and drawing pattern (Naeem 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, vaporizaton 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).

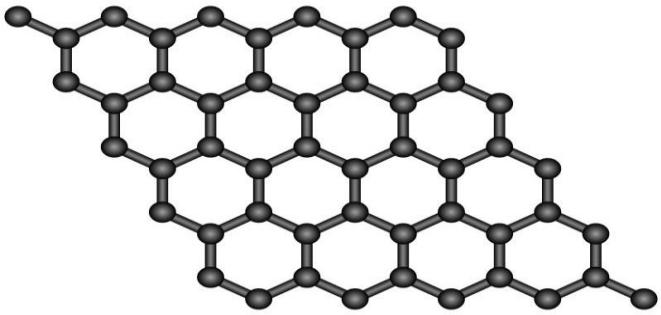
In this paper, we will discuss Magnesium Oxide (111) for $s = 1,2,3,\dots s$. Figure 1 is the molecular structure of MgO(111). The crystal structure of Magnesium Oxide MgO(111) contains the $2(4s^2 + 4s + 1)$ vertices and $12s^2 + 8s + 1$ edges.

Table 1: Ev-degrees and Ve-degree indices

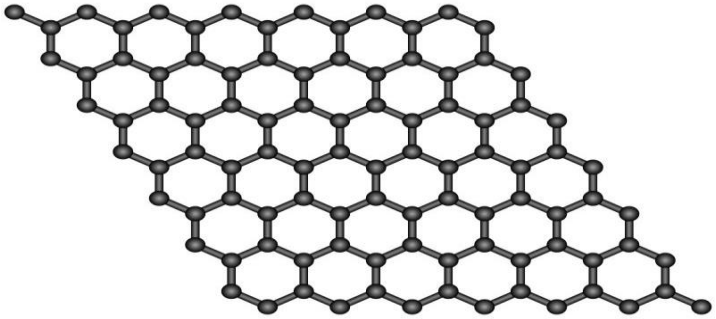
Ev-degree based topological indices	**Notation**	**Numerical equation**
Randić index	R^{ev}	$\sum_{e\in E} \aleph_{ev}(e)^{-\frac{1}{2}}$
Zagreb index	M^{ev}	$\sum_{e\in E} \aleph_{ev}(e)^2$
Ve-degree based topological indices	**Notation**	**Mathematical Formula**
First Zagreb β-index	$M_1^{\beta ve}$	$\sum_{uv\in E} [\aleph_{ve}(u) + \aleph_{ve}(v)]$
Second Zagreb β-index	$M_2^{\beta ve}$	$\sum_{uv\in E} [\aleph_{ve}(u) \times \aleph_{ve}(v)]$
Harmonic index	H^{ve}	$\sum_{uv\in E} \frac{2}{\aleph_{ve}(u)+\aleph_{ve}(v)}$
Sum Connectivity index	χ^{ve}	$\sum_{uv\in E} [\aleph_{ve}(u) + \aleph_{ve}(v)]^{-\frac{1}{2}}$
Geometric Arithmetic index	GA^{ve}	$\sum_{uv\in E} \frac{2\sqrt{\aleph_{ve}(u)\times\aleph_{ve}(v)}}{(\aleph_{ve}(u)+\aleph_{ve}(v))}$
Atom Bond Connectivity index	ABC^{ve}	$\sum_{uv\in E} \sqrt{\frac{\aleph_{ve}(u)+\aleph_{ve}(v)-2}{(\aleph_{ve}(u)\times\aleph_{ve}(v))}}$
Randić index	R^{ve}	$\sum_{uv\in E} [\aleph_{ve}(u) \times \aleph_{ve}(v)]^{-\frac{1}{2}}$
First Zagreb α-index	$M_1^{\alpha ve}$	$\sum_{v\in V(H)} \aleph_{ve}(v)^2$



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

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

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

$$\mathrm{M}^{ev}(H) = \sum_{e\in E(H)} \aleph_{ev}(e)^2,$$
$$\mathrm{M}^{ev}(H) = (3)^2|E_{(1,2)}| + (4)^2|E_{(2,2)}| + (5)^2|E_{(2,3)}| + (6)^2|E_{(3,3)}|$$
$$= 2\times 9 + 4\times 16 + (16s-4)\times 25 + (4s(3s-2)+1)\times 36$$
$$= 432s^2 + 112s + 18.$$

(b) The ev-degree Randić index

$$\mathrm{R}^{ev}(H) = \sum_{e\in E(H)} \aleph_{ev}(e)^{-\frac{1}{2}},$$
$$\mathrm{R}^{ev}(H) = (3)^{-\frac{1}{2}}|E_{(1,2)}| + (4)^{-\frac{1}{2}}|E_{(2,2)}| + (5)^{-\frac{1}{2}}|E_{(2,3)}| + (6)^{-\frac{1}{2}}|E_{(3,3)}|$$
$$= 2\times (3)^{-\frac{1}{2}} + 4\times (4)^{-\frac{1}{2}} + 4(4s-1)\times (5)^{-\frac{1}{2}} + (12s^2-8s+1)\times (6)^{-\frac{1}{2}}$$
$$= \frac{12}{\sqrt{6}}s^2 + \left(\frac{16}{\sqrt{5}} - \frac{8}{\sqrt{6}}\right)s + \left(\frac{2}{\sqrt{3}} + 2 - \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right).$$

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

$(\aleph(u), \aleph(v))$	$\aleph_{ev}(e)$	**Frequency**
$E_{(1,2)}$	3	2
$E_{(2,2)}$	4	4
$E_{(2,3)}$	5	$4(4s-1)$
$E_{(3,3)}$	6	$4s(3s-2)+1$

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 α-index is designated*

$$\mathrm{M}_1^{\alpha ve}(H) = 648s^2 + 32s - 20.$$

Proof 2 *via structure of MgO(111), we partitioned the vertices into six seperations 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)

$\aleph(u)$	$\aleph_{ve}(u)$	**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 α-index.

$$\mathrm{M}_1^{\alpha ve}(H) = \sum_{v \in V(H)} \aleph_{ve}(v)^2$$

$$\mathrm{M}_1^{\alpha ve}(H) = 2 \times (2)^2 + 4 \times (5)^2 + 4(2s-1) \times (6)^2 + 2 \times (5)^2 + 4(2s-1) \times (7)^2 + 2(4s^2 - 4s + 1) \times (9)^2 = 648s^2 + 32s - 20.$$

Numerical Computation of the Ve-degree based first Zagreb alpha index ($M_1^{\alpha ve}$) 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 Randic kind of indices. Ediz tested in such a way that $M_1^{\alpha ve}$ 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^{ev}) is weaker predictor of molecular mass than $M_1^{\alpha ve}$. 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) $\mathrm{M}_1^{\beta ve}(H) = 216s^2 + 48s - 2.$

(b) $\mathrm{M}_2^{\beta ve}(H) = 972s^2 - 120s - 11.$

(c) $\mathrm{ABC}^{ve}(H) = 4\sqrt{2}s^2 + (\frac{16\sqrt{13}}{\sqrt{42}} + \frac{32}{3\sqrt{7}} - \frac{16\sqrt{2}}{3})s + (\frac{2\sqrt{2}}{\sqrt{5}} + \frac{4\sqrt{2}}{5} + \frac{4\sqrt{11}}{\sqrt{30}} + \frac{8\sqrt{3}}{\sqrt{35}} - \frac{12\sqrt{13}}{\sqrt{42}} - \frac{16}{3\sqrt{7}} + \frac{5\sqrt{2}}{3}).$

(d) $\mathrm{GA}^{ve}(H) = 12s^2 + (\frac{32\sqrt{42}}{13} + 3\sqrt{7} - 16)s + (\frac{\sqrt{15}}{2} + \frac{8\sqrt{30}}{11} + \frac{2\sqrt{35}}{3} - \frac{24\sqrt{42}}{13} - \frac{3\sqrt{7}}{2} + 7).$

(e) $\mathrm{H}^{ve}(H) = \frac{4}{3}s^2 + (\frac{32}{13} - \frac{16}{9} + 1)s + (\frac{2}{5} + \frac{8}{11} - \frac{24}{13} + \frac{2}{3} + \frac{5}{6}).$

(f) $\chi^{ve}(H) = \frac{4}{\sqrt{2}}s^2 + (\frac{16}{\sqrt{13}} - \frac{16}{\sqrt{18}} + 2)s + (\frac{1}{\sqrt{2}} + \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{4}{\sqrt{12}} + \frac{5}{\sqrt{18}} - \frac{12}{\sqrt{13}} - 1).$

(g) $\mathrm{R}^{ve}(H) = \frac{4}{3}s^2 + (\frac{16}{\sqrt{42}} + \frac{8}{3\sqrt{7}} - \frac{16}{9})s + (\frac{2}{\sqrt{15}} + \frac{2}{5} - \frac{4}{\sqrt{30}} + \frac{4}{\sqrt{35}} - \frac{12}{\sqrt{42}} - \frac{4}{3\sqrt{7}} + \frac{5}{9}).$

Proof 3 *To calculate the Ve degree indices, we must first determine the point seperation of* $E(H)$

dependent on the Ve degree of all edge's peak vertices. This seperation 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	$(\aleph_{ve}(u), \aleph_{ve}(v))$	**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 β-index

$$\mathrm{M}_1^{\beta ve}(H) = \sum_{uv\in E(H)} (\aleph_{ve}(u) + \aleph_{ve}(v))$$

$$\begin{aligned}\mathrm{M}_1^{\beta ve}(H) &= (8)|E_1^*| + (10)|E_2^*| + (11)|E_3^*| + (12)|E_4^*| + (13)|E_5^*| + (16)|E_6^*| + (18)|E_7^*| \\ &= 2\times 8 + 2\times 10 + 4\times 11 + 4\times 12 + 4(4s-3)\times 13 + 4(2s-1)\times 16 \\ &+(12s^2-16s+5)\times 18 \\ &= 216s^2+48s-2.\end{aligned}$$

(b) The second Zagreb β-index

$$\mathrm{M}_2^{\beta ve}(H) = \sum_{uv\in E(H)} (\aleph_{ve}(u) \times \aleph_{ve}(v))$$

$$\begin{aligned}\mathrm{M}_2^{\beta ve}(H) &= (15)|E_1^*| + (25)|E_2^*| + (30)|E_3^*| + (35)|E_4^*| + (42)|E_5^*| + (63)|E_6^*| + (81)|E_7^*| \\ &= 2\times 15 + 2\times 25 + 4\times 30 + 4\times 35 + 4(4s-3)\times 42 + 4(2s-10)\times 63 \\ &+(12s^2-16s+5)\times 81 \\ &= 972s^2-120s-11.\end{aligned}$$

(c) The Atom-bond connectivity index

$$\mathrm{ABC}^{ve}(H) = \sum_{uv\in E(H)} \sqrt{\frac{\aleph_{ve}(u)+\aleph_{ve}(v)-2}{(\aleph_{ve}(u)\times\aleph_{ve}(v))}}$$

$$\begin{aligned}\mathrm{ABC}^{ve}(H) &= (\sqrt{\tfrac{2}{15}})|E_1^*| + (\sqrt{\tfrac{8}{25}})|E_2^*| + (\sqrt{\tfrac{11}{30}})|E_3^*| + (\sqrt{\tfrac{12}{35}})|E_4^*| + (\sqrt{\tfrac{13}{42}})|E_5^*| \\ &+(\sqrt{\tfrac{16}{63}})|E_6^*| + (\sqrt{\tfrac{18}{81}})|E_7^*| \\ &= 2\times\sqrt{\tfrac{2}{15}} + 2\times\sqrt{\tfrac{8}{25}} + 4\times\sqrt{\tfrac{11}{30}} + 4\times\sqrt{\tfrac{12}{35}} + 4(4s-3)\times\sqrt{\tfrac{13}{42}} \\ &+4(2s-1)\times\sqrt{\tfrac{16}{63}} + (12s^2-16s+5)\times\sqrt{\tfrac{18}{81}} \\ &= 4\sqrt{2}s^2 + (\tfrac{16\sqrt{13}}{\sqrt{42}} + \tfrac{32}{3\sqrt{7}} - \tfrac{16\sqrt{2}}{3})s + (\tfrac{2\sqrt{2}}{\sqrt{5}} + \tfrac{4\sqrt{2}}{5} + \tfrac{4\sqrt{11}}{\sqrt{30}} + \tfrac{8\sqrt{3}}{\sqrt{35}} \\ &-\tfrac{12\sqrt{13}}{\sqrt{42}} - \tfrac{16}{3\sqrt{7}} + \tfrac{5\sqrt{2}}{3}).\end{aligned}$$

(d) The Geometric-arithmetic index

$$\mathrm{GA}^{ve}(H) = \sum_{uv\in E(H)} \frac{2\sqrt{\aleph_{ve}(u)\times\aleph_{ve}(v)}}{(\aleph_{ve}(u)+\aleph_{ve}(v))}$$

$$\mathrm{GA}^{ve}(H) = (\frac{2\sqrt{15}}{8})|E_1^*| + (\frac{2\sqrt{25}}{10})|E_2^*| + (\frac{2\sqrt{30}}{11})|E_3^*| + (\frac{2\sqrt{35}}{12})|E_4^*| + (\frac{2\sqrt{42}}{13})|E_5^*|$$
$$+(\frac{2\sqrt{63}}{16})|E_6^*| + (\frac{2\sqrt{81}}{18})|E_7^*|$$
$$= 2\times\frac{2\sqrt{15}}{8} + 2\times\frac{2\sqrt{25}}{10} + 4\times\frac{2\sqrt{30}}{11} + 4\times\frac{2\sqrt{35}}{12} + 4(4s-3)\times\frac{2\sqrt{42}}{13}$$
$$+4(2s-1)\times\frac{2\sqrt{63}}{16} + (12s^2-16s+5)\times\frac{2\sqrt{81}}{18}$$
$$= 12s^2 + (\frac{32\sqrt{42}}{13} + 3\sqrt{7} - 16)s + (\frac{\sqrt{15}}{2} + \frac{8\sqrt{30}}{11} + \frac{2\sqrt{35}}{3} - \frac{24\sqrt{42}}{13} - \frac{3\sqrt{7}}{2} + 7).$$

(e) The Harmonic index

$$\mathrm{H}^{ve}(H) = \sum_{uv\in E(H)} \frac{2}{\aleph_{ve}(u)+\aleph_{ve}(v)}$$

$$\mathrm{H}^{ve}(H) = (\frac{2}{8})|E_1^*| + (\frac{2}{10})|E_2^*| + (\frac{2}{11})|E_3^*| + (\frac{2}{12})|E_4^*| + (\frac{2}{13})|E_5^*| + (\frac{2}{16})|E_6^*| + (\frac{2}{18})|E_7^*|$$
$$= 2\times\frac{2}{8} + 2\times\frac{2}{10} + 4\times\frac{2}{11} + 4\times\frac{2}{12} + 4(4s-3)\times\frac{2}{13} + 4(2s-1)\times\frac{2}{16}$$
$$+(12s^2-16s+5)\times\frac{2}{18}$$
$$= \frac{4}{3}s^2 + (\frac{32}{13} - \frac{16}{9} + 1)s + (\frac{2}{5} + \frac{8}{11} - \frac{24}{13} + \frac{2}{3} + \frac{5}{6}).$$

(f) The Sum-connectivity index

$$\chi^{ve}(H) = \sum_{uv\in E(H)} (\aleph_{ve}(u) + \aleph_{ve}(v))^{-\frac{1}{2}}$$

$$\chi^{ve}(H) = (8)^{-\frac{1}{2}}|E_1^*| + (10)^{-\frac{1}{2}}|E_2^*| + (11)^{-\frac{1}{2}}|E_3^*| + (12)^{-\frac{1}{2}}|E_4^*| + (13)^{-\frac{1}{2}}|E_5^*| + (16)^{-\frac{1}{2}}|E_6^*|$$
$$+(18)^{-\frac{1}{2}}|E_7^*|$$
$$= \frac{2}{\sqrt{8}} + \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{4}{\sqrt{12}} + \frac{4(4s-3)}{\sqrt{13}} + \frac{4(2s-1)}{\sqrt{16}} + \frac{(12s^2-16s+5)}{\sqrt{18}}$$
$$= \frac{4}{\sqrt{2}}s^2 + (\frac{16}{\sqrt{13}} - \frac{16}{\sqrt{18}} + 2)s + (\frac{1}{\sqrt{2}} + \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{4}{\sqrt{12}} + \frac{5}{\sqrt{18}} - \frac{12}{\sqrt{13}} - 1).$$

(g) The Randić index

$$\mathrm{R}^{ve}(H) = \sum_{uv\in E(H)} (\aleph_{ve}(u) \times \aleph_{ve}(v))^{-\frac{1}{2}}$$

$$\mathrm{R}^{ve}(H) = (15)^{-\frac{1}{2}}|E_1^*| + (25)^{-\frac{1}{2}}|E_2^*| + (30)^{-\frac{1}{2}}|E_3^*| + (35)^{-\frac{1}{2}}|E_4^*| + (42)^{-\frac{1}{2}}|E_5^*| + (63)^{-\frac{1}{2}}|E_6^*|$$
$$+(81)^{-\frac{1}{2}}|E_7^*|$$
$$= 2\times(15)^{-\frac{1}{2}} + 2\times(25)^{-\frac{1}{2}} + 4\times(30)^{-\frac{1}{2}} + 4\times(35)^{-\frac{1}{2}} + 4(4s-3)\times(42)^{-\frac{1}{2}}$$
$$+4(2s-1)\times(63)^{-\frac{1}{2}} + (12s^2-16s+5)\times(81)^{-\frac{1}{2}}$$
$$= \frac{4}{3}s^2 + (\frac{16}{\sqrt{42}} + \frac{8}{3\sqrt{7}} - \frac{16}{9})s + (\frac{2}{\sqrt{15}} + \frac{2}{5} - \frac{4}{\sqrt{30}} + \frac{4}{\sqrt{35}} - \frac{12}{\sqrt{42}} - \frac{4}{3\sqrt{7}} + \frac{5}{9}).$$

Numerical Computation of the index values relying upon Ve-degree of terminal vertices of every edge exhibits a stadily 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 ($M_1^{\beta ve}$) foretells the molecular mass and Topographical Polar area greater than other Ve-degree of

peak vertices dependent index values. In general, $M_1^{\beta ve}$ 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 π −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 π −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	$\mathbf{M}^{ev}$	$\mathbf{M}_1^{\alpha ve}$	$\mathbf{M}_1^{\beta ve}$	$\mathbf{M}_2^{ve}$	$\mathbf{R}^{ve}$
[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	$\mathbf{R}^{ev}$	$\mathbf{ABC}^{ve}$	$\mathbf{GA}^{ve}$	$\mathbf{H}^{ve}$	$\boldsymbol{\chi}^{ve}$
[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	112.898167	255.241388	28.849495	71.555859
[5]	321.055404	11.873172	376.51198	42.533256	103.449304
[6]	456.944836	34.234462	521.7825623	58.883683	140.999604
[7]	616.834267	67.9094599	691.0531498	77.90078	184.206759
[8]	800.723698	112.898167	884.323737	99.5845377	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 increases for MgO(111) structure. Different sorts of graphical constants have been elaborated and examined , pressenting 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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