Research Article

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On ve-degree- and ev-degree-based topological properties of crystallographic structure of cuprite Cu_2O

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Abstract: In the study of chemical graph theory, an enormous number of research analyses have confirmed that the characteristics of chemicals have a nearby connection with their atomic structure. Topological indices were the critical tools for the analysis of these chemical substances to consider the essential topology of chemical structures. Topological descriptors are the significant numerical quantities or invariant in the fields of chemical graph theory. In this study, we have studied the crystal structure of copper oxide (Cu_2O) chemical graph, and further, we have calculated the ev-degree- and ve-degree-based topological indices of copper oxide chemical graph. This kind of study may be useful for understanding the atomic mechanisms of corrosion and stress–corrosion cracking of copper.

Keywords: ev-degree, ve-degree, topological indices, cuprite Cu_2O

MSC 2020: 05C09, 05C92, 92E10

1 Introduction

The chemical graph theory, a field of graph theory, offers a wide range of opportunities for mathematical chemists. In chemistry, several chemical compounds having the same chemical formula but different in structure and in molecular graph theory vertices represent atoms, and edges represent bonds in a molecular graph. In the field of chemistry, topological theories have also been used; the topology defines the shape of prominent Huckel molecular orbitals (HMOs). The degree of vertex is usually referred to in the chemical graph for its valence. The formation of several modern scientific principles and their uses in various branches of chemistry are now the key focus of the graph theory. A quick study of quantitative structure–property or structure–activity relationships (QSPR/QSAR) is one of the key reasons for extending the graph theory to chemistry [1,2]. Researchers are interested to work on the topology of a chemical network associated with medical research, drug, medicine, and experimental science using certain mathematical tools obtained from the molecular structures of these networks in the QSPR/QSAR analyses [3]. The development of the topological theory of chemistry allows chemists to think as far as possible about the molecules' and their chemical behavior by examining their molecular graph characteristics. The topological indices have been used to develop and understand the mathematical characteristics of the real-world network model on a wide range of topics related to bioinformatics and proteomics.

First, Wiener presented the topological descriptor [4] and found the first index name as the Wiener index also known as *path number*. An oldest topological index names as Randic-type index was introduced by Randic [5] in 1975.

Topological indices used for mathematical and chemical literature are Wiener, Randic, and Zagreb indices [4–6]. In 1998, the idea about generalized Randic index was given by Erdos and Ballobas, and Amic et al., see [7,8].

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The Randic index is by far the most prominent, most frequently used and studied topological index of all others. Gutman and Trinajstić were given the concept of first Zagreb-type index, the second Zagreb-type index, and the second-modified Zagreb-type index [9–11]. The Randic index variant is the harmonic index. Harmonic index was defined by Zhong [12], and later, novel Harmonic indices were defined by Ediz et al. [13]. However, all research works were performed by utilizing the classical concept of degrees.

In the graph theory, Chellali et al. [14] recently published two novel degree-based definitions, namely *ev-degree* and *ve-degree*. Horoldagva et al. [15] later explored some of the *ev-degree* and *ve-degree* concepts associated with mathematical principles. The classical definition of degrees was transformed into *ev-degree* and *ve-degree*. In this study, we have presented a few initial ideologies of *ve-degree* and *ev-degree*, and we have calculated the *ev-degree*- and *ve-degree*-based topological indices for the chemical structure of copper oxide.

Definitions

The **ev-degree** of any edge $uv = e \in E(G)$ is the total quantity of the vertices set of the union of the u and v closed neighborhoods, the *ev degree* is denoted by $\Lambda_{ev}(e)$.

The **ve-degree** of any vertex $v \in V(G)$ is the total quantity of those edges that are incident to any vertices from the closed neighborhood of v , i.e., the sum of all closed neighborhood vertex degrees of v .

ev-degree-based indices

For a connected graph G , the *ev-degree*-based Zagreb (M^{ev}) index and Randic (R^{ev}) index for any edge $e = uv \in E(G)$ are defined as

$$M^{ev}(G) = \sum_{e \in E} \Lambda_{ev}(e)^2, \quad R^{ev}(G) = \sum_{e \in E} \Lambda_{ev}(e)^{-\frac{1}{2}}.$$

ve-degree-based indices

For a connected graph G , the *ve-degree*-based first Zagreb alpha (M_1^{ave}) index for any vertex $v \in V(G)$ is defined as

$$M_1^{ave}(G) = \sum_{v \in V} \Lambda_{ve}(v)^2.$$

End vertex ve-degree-based indices of each edge

For a connected graph G , the end vertices *ve-degree*-based indices for each edges, such as *ve-degree*-based first Zagreb beta ($M_1^{\beta ve}$) index, second Zagreb ($M_2^{\beta ve}$) index, atom-bond connectivity (ABC^{ve}) index, geometric-arithmetic (GA^{ve}) index, Harmonic (H^{ve}) index, sum-connectivity (χ^{ve}) index, and the Randic (R^{ve}) index for each edge $uv \in E(G)$ are defined as

$$\begin{aligned} M_1^{\beta ve}(G) &= \sum_{uv \in E} (\Lambda_{ve}(u) + \Lambda_{ve}(v)), \\ M_2^{\beta ve}(G) &= \sum_{uv \in E} (\Lambda_{ve}(u) \times \Lambda_{ve}(v)), \\ ABC^{ve}(G) &= \sum_{uv \in E} \sqrt{\frac{\Lambda_{ve}(u) + \Lambda_{ve}(v) - 2}{\Lambda_{ve}(u) \times \Lambda_{ve}(v)}}, \\ GA^{ve}(G) &= \sum_{uv \in E} \frac{2\sqrt{\Lambda_{ve}(u) \times \Lambda_{ve}(v)}}{\Lambda_{ve}(u) + \Lambda_{ve}(v)}, \\ H^{ve}(G) &= \sum_{uv \in E} \frac{2}{\Lambda_{ve}(u) + \Lambda_{ve}(v)}, \\ \chi^{ve}(G) &= \sum_{uv \in E} (\Lambda_{ve}(u) + \Lambda_{ve}(v))^{-\frac{1}{2}}, \\ R^{ve}(G) &= \sum_{uv \in E} (\Lambda_{ve}(u) \times \Lambda_{ve}(v))^{-\frac{1}{2}}. \end{aligned}$$

2 Methodology

Mathematica was used for computing results for *ev-degree*, *ve-degree*, and *ve-degree* of the end vertices of each edge. Matlab was used for the calculation and verification of results. Maple was used for graphical representation of these results obtained from.

Ethical approval: The conducted research is not related to either human or animal use.

3 Copper oxide (Cu_2O)

Cuprite is the oldest semiconductor electronic material. It has been the focus of various experimental and theoretical studies but the researchers remain perplexed by its electronic and atomic structure. Copper oxide (Cu_2O) is a commonly occurred copper corrosion product, and new applications of Cu_2O in nanoelectronics, photovoltaics, and spintronics are emerging. To predict and control the actions of copper corrosion, understanding cuprite at the level of electronic and atomic structure can be helpful.

Cuprite is a deficient metal with an extrinsic semiconductor p-type having basic structural paradigm properties based on the presence of cation vacancy as a prevalent ionic deficiency at sufficiently high temperatures and oxygen activity [16]. Cuprite nonstoichiometry was studied using gas volumetric analysis by Dünwald and Wagner in 1933 [17], quenched sample chemical analysis by Wagner and Hammen in 1938 [18], and thermogravimetry by O'Keeffe and Moore in 1962 [19]. At temperatures

Figure 1: (a) Copper oxide (Cu_2O) structural features where Cu are copper and O are oxygen atoms and (b) unit cell of copper oxide (Cu_2O) lattice.

between 300 and 1,000 °C, Park and Natesan [20] studied thermogravimetric oxidation of copper in air and oxygen. Wang et al. [21] conducted a theoretical analysis on the impact of pH on cuprite's defect structure and transportation properties, which is synthesized from an aqueous solution.

3.1 Crystallographic structure of copper oxide

The properties of copper oxide such as non-poisonous nature, plenitude, ease, and simple assembling measure; Cu_2O have attracted considerable attention among various transition metal oxides in recent years [22]. Today, Cu_2O 's promising applications are centered principally around

compound sensors, sunlight-based cells, photocatalysis, lithium-particle batteries, and catalysis [23]. Figures 1 and 2 portray that the substance diagram of Cu_2O , which is a crystallographic structure, see data in [24,25]. Copper oxide (Cu_2O) primary highlights where Cu are copper and O are oxygen atoms. The Cu_2O grid is shaped by interpenetrating the Cu and O molecules, see Figure 1a. Unit cell of Cu_2O cross-section is shown in Figure 1b. As little blue circles, copper molecules are depicted, and oxygen particles are shown as large red circles. Inside the Cu_2O grid, each Cu_2O particle is composed of two O atoms, and every O molecule is facilitated with four Cu atoms.

The Cu_2O lattice developed in the $p \times q$ plane and accumulated it in r layers, see Figure 2. The crystal structure of Cu_2O contains the $1 + p + q + pq + r + pr + qr + 6pqr$ vertices and $8pqr$ edges, respectively. On the base of degrees, the vertices of Cu_2O divides into four partitions in such a way; four vertices of degree zero, $4p + 4q + 4r - 8$ vertices of degree one, $2(pq + pr + qr - 2p - 2q - 2r + 3)$ vertices of degree 2, and $2pqr - pq - qr - pr + q + p + r - 1$ vertices of degree four. Similarly, the edges of Cu_2O are partitioned as $E_{(1,2)}$ with $4(p + q + r - 2)$ edges, $E_{(2,2)}$ with $2(pq + pr + qr - 2p - 2q - 2r + 3)$ edges, and $E_{(2,4)}$ having $8pqr - 4pq - 4pr - 4qr + 4p + 4q + 4r - 4$.

4 Main results

Theorem 1. Let G be a molecular graph of cuprite Cu_2O , then *ev-degree-based Zagreb index* and *ev-degree-based Randic index* are given by,

Figure 2: (a) Unit cell of $\text{Cu}_2\text{O}[1, 1, 1]$ and (b) the crystallographic structure of $\text{Cu}_2\text{O}[3, 2, 3]$.

$$(a) \quad M^{\text{ev}}(G) = 116(p + q + r) - 112(pq - pr - qr) + 288pqr - 120$$

(b)

$$\begin{aligned} R^{\text{ev}}(G) = & \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)p + \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)q \\ & + \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)r + \left(1 - \frac{4}{\sqrt{6}}\right)pq + \left(1 - \frac{4}{\sqrt{6}}\right)pr \\ & + \left(1 - \frac{4}{\sqrt{6}}\right)qr + \frac{4}{3}pqr - \left(\frac{8}{\sqrt{3}} + \frac{4}{\sqrt{6}} - 3\right) \end{aligned}$$

Proof. From the structure of Cu_2O , we divide the edges into three partitions $E_{(1,2)}$, $E_{(2,2)}$ and $E_{(2,4)}$ respectively, where the total quantity of the edges are $8pqr$. By the definition of ev-degree, we have calculated the ev-degrees of the given edges partition as shown in Table 1. $\square$

From Table 1, we have proved ev-degree-based indices such as:

(a) The ev-degree-based Zagreb index:

$$\begin{aligned} M^{\text{ev}}(G) &= \sum_{e \in E(G)} \Lambda_{\text{ev}}(e)^2, \\ M^{\text{ev}}(G) &= (3)^2|E_{(1,2)}| + (4)^2|E_{(2,2)}| + (6)^2|E_{(2,4)}| \\ &= 9(4p + 4q + 4r - 8) + 16[2(pq + pr + qr - 2p - 2q - 2r + 3)] + 36(8pqr - 4pq - 4pr - 4qr + 4p + 4q + 4r - 4) \\ &= 116(p + q + r) - 112(pq - pr - qr) + 288pqr - 120. \end{aligned}$$

(b) The ev-degree-based Randic index:

$$\begin{aligned} R^{\text{ev}}(G) &= \sum_{e \in E(G)} \Lambda_{\text{ev}}(e)^{-\frac{1}{2}}, \\ R^{\text{ev}}(G) &= (3)^{-\frac{1}{2}}|E_{(1,2)}| + (4)^{-\frac{1}{2}}|E_{(2,2)}| + (6)^{-\frac{1}{2}}|E_{(2,4)}| \\ &= (3)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (4)^{-\frac{1}{2}}[2(pq + pr + qr - 2p - 2q - 2r + 3)] + (6)^{-\frac{1}{2}}(8pqr - 4pq - 4pr - 4qr + 4p + 4q + 4r - 4) \\ &= \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)p + \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)q \\ &\quad + \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)r + \left(1 - \frac{4}{\sqrt{6}}\right)pq \\ &\quad + \left(1 - \frac{4}{\sqrt{6}}\right)pr + \left(1 - \frac{4}{\sqrt{6}}\right)qr \\ &\quad + \frac{4}{3}pqr - \left(\frac{8}{\sqrt{3}} + \frac{4}{\sqrt{6}} - 3\right). \end{aligned}$$

Table 1: The edges ev-degree of Cu_2O

$(\Lambda(u), \Lambda(v))$	$\Lambda_{\text{ev}}(e)$	Frequency
$E_{(1,2)}$	3	$4p + 4q + 4r - 8$
$E_{(2,2)}$	4	$2(pq + pr + qr - 2p - 2q - 2r + 3)$
$E_{(2,4)}$	6	$8pqr - 4pq - 4pr - 4qr + 4p + 4q + 4r - 4$

Theorem 2. Let G be a molecular graph of cuprite Cu_2O , then vertices ve-degree-based first Zagreb α -index is given by,

$$M_1^{\alpha\text{ve}}(G) = 84(p + q + r) - 144(pq + pr + qr) + 384pqr - 24$$

Proof. From the structure of Cu_2O , we divide the vertices into four partitions on the bases of degrees V_0 , V_1 , V_2 , and V_4 respectively, where the total quantity of the vertices are $6pqr + pq + qr + pr + q + p + r + 1$. By the definition of ve-degrees, we have calculated the vertices ve-degrees as shown in Table 2. $\square$

By using Table 2, we have first calculated ve-degree-based Zagreb α -index (Figures 3 and 4).

$$\begin{aligned} M_1^{\alpha\text{ve}}(G) &= \sum_{v \in V(G)} \Lambda_{\text{ve}}(v)^2, \\ M_1^{\alpha\text{ve}}(G) &= (0)^2(4) + (2)^2(4p + 4q + 4r - 8) \\ &\quad + (4)^2(2pq + 2pr + 2qr - 4p - 4q - 4r + 6) \\ &\quad + (5)^2(4p + 4q + 4r - 8) + (6)^2(4pq + 4pr + 4qr - 4p - 4q - 4r + 12) \\ &\quad + (8)^2[4(q - 1)(p - 1)(r - 1)] \\ &\quad + (8)^2(2pqr - pq - qr - pr + q + p + r - 1) \\ &= 84(q + p + r) - 144(pq + qr + pr) + 384pqr - 24. \end{aligned}$$

Theorem 3. Let G be a molecular graph of cuprite Cu_2O , then end vertices ve-degree-based indices of each edges are given by,

$$\begin{aligned} (a) \quad M_1^{\beta\text{ve}}(G) &= 112(q + p + r) - 80(pq + qr + pr) + 128pqr - 144 \\ (b) \quad M_2^{\beta\text{ve}}(G) &= 424(q + p + r) - 368(pq - qr - pr) + 512pqr + 136 \end{aligned}$$

Table 2: The vertices ve-degrees of Cu_2O

$\Lambda(u)$	$\Lambda_{\text{ve}}(u)$	Frequency
0	0	4
1	2	$4(p + q + r - 2)$
2	4	$2pq + 2pr + 2qr - 4p - 4q - 4r + 6$
2	5	$4p + 4q + 4r - 8$
2	6	$4pq + 4pr + 4qr - 4p - 4q - 4r + 12$
2	8	$4(q - 1)(p - 1)(r - 1)$
4	8	$2pqr - pq - qr - pr + q + p + r - 1$

$$\begin{aligned}
\text{(c) } ABC^{ve}(G) &= \left(\frac{4}{\sqrt{2}} - \frac{4}{\sqrt{3}} + 2\sqrt{\frac{11}{10}} \right) [p + q + r] \\
&\quad + \left(\frac{2}{\sqrt{3}} + 1 - \sqrt{14} \right) [pq + pr + qr] \\
&\quad + \sqrt{14}pqr + \left(2\sqrt{3} + \sqrt{14} + 7 - 4\sqrt{\frac{11}{10}} \right) \\
\text{(d) } GA^{ve}(G) &= 8 \left(\frac{\sqrt{10}}{7} + \frac{\sqrt{6}}{5} + \frac{2\sqrt{10}}{13} + \frac{2\sqrt{3}}{7} + 1 \right) [p + q + r] \\
&\quad + 4 \left(\frac{\sqrt{6}}{5} + \frac{2\sqrt{3}}{7} + 2 \right) [pq + pr + qr] + 8pqr \\
&\quad + \left(8 + \frac{12\sqrt{6}}{5} - \frac{16\sqrt{10}}{7} - \frac{32\sqrt{10}}{13} + \frac{24\sqrt{3}}{7} \right) \\
\text{(e) } H^{ve}(G) &= \frac{631}{455}(p + q + r) + \frac{59}{35}(pq + pr + qr) + pqr + \frac{209}{455} \\
\text{(f) } \chi^{ve}(G) &= 4 \left(\frac{1}{\sqrt{7}} - \frac{1}{\sqrt{10}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{14}} + 1 \right) [p + q + r] \\
&\quad + \left(\frac{2}{\sqrt{10}} + \frac{2}{\sqrt{14}} + 4 \right) [pq + pr + qr] + 4pqr \\
&\quad + \left(\frac{6}{\sqrt{10}} - \frac{8}{\sqrt{7}} - \frac{8}{\sqrt{13}} + \frac{6}{\sqrt{14}} + 4 \right) \\
\text{(g) } R^{ve}(G) &= \left(\frac{6}{\sqrt{10}} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}} + 1 \right) [p + q + r] \\
&\quad + \left(\frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{3}} - 1 \right) [pq + pr + qr] + pqr \\
&\quad + \left(\frac{-12}{\sqrt{10}} + \frac{3}{\sqrt{6}} - \frac{\sqrt{3}}{2} - 1 \right)
\end{aligned}$$

Proof. From the structure of Cu_2O , we divide the edges into three partitions $E_{(1,2)}$, $E_{(2,2)}$, and $E_{(2,4)}$ respectively, where the total quantity of the edges is $8pqr$. By the definition of end vertices ve-degree of each edge, we divide the new edges into five partitions, i.e., E_1^* , E_2^* , E_3^* , E_4^* , and E_5^* respectively, as shown in Table 3. $\square$

By using the table, we can prove end vertices ve-degree-based indices of each edge such as (Figures 5–8),

(a) The first Zagreb β -index:

(a)

Figure 4: The first Zagreb α -index.

$$\begin{aligned}
M_1^{\beta ve}(G) &= \sum_{uv \in E(G)} (\Lambda_{ve}(u) + \Lambda_{ve}(v)), \\
M_1^{\beta ve}(G) &= (7)|E_1^*| + (10)|E_2^*| + (13)|E_3^*| \\
&\quad + (14)|E_4^*| + (16)|E_5^*| \\
&= (7)(4p + 4q + 4r - 8) + (10)(2pq + 2pr \\
&\quad + 2qr - 4p - 4q - 4r + 12) \\
&\quad + (13)(4p + 4q + 4r - 8) + (14)(2pq + 2pr \\
&\quad + 2qr - 4p - 4q - 4r + 12) \\
&\quad + (16)[8(q - 1)(p - 1)(r - 1)] \\
&= 112(q + p + r) - 80(pq + qr + pr) \\
&\quad + 128pqr - 144.
\end{aligned}$$

(b) The second Zagreb β -index:

$$\begin{aligned}
M_2^{\beta ve}(G) &= \sum_{uv \in E(G)} (\Lambda_{ve}(u)\Lambda_{ve}(v)), \\
M_2^{\beta ve}(G) &= (10)|E_1^*| + (24)|E_2^*| + (40)|E_3^*| \\
&\quad + (48)|E_4^*| + (64)|E_5^*| \\
&= (10)(4p + 4q + 4r - 8) + (24)(2pq + 2pr \\
&\quad + 2qr - 4p - 4q - 4r + 12) \\
&\quad + (40)(4p + 4q + 4r - 8) + (48)(2pq + 2pr \\
&\quad + 2qr - 4p - 4q - 4r + 12) \\
&\quad + (64)[8(q - 1)(p - 1)(r - 1)] \\
&= 424(q + p + r) - 368(pq + qr + pr) \\
&\quad + 512pqr + 136.
\end{aligned}$$

(b)

Figure 3: The ev-degree-based indices: (a) the Zagreb index and (b) the Randic index.

Table 3: Ve-degrees of end vertices of each edge of Cu_2O

Edge	$(\Lambda_{ve}(u), \Lambda_{ve}(v))$	Frequency
E_1^*	(2, 5)	$4p + 4q + 4r - 8$
E_2^*	(4, 6)	$2pq + 2pr + 2qr - 4p - 4q - 4r + 12$
E_3^*	(5, 8)	$4(p + q + r - 2)$
E_4^*	(6, 8)	$2pq + 2pr + 2qr - 4p - 4q - 4r + 12$
E_5^*	(8, 8)	$8(q - 1)(p - 1)(r - 1)$

(c) The atom-bond connectivity index:

$$\begin{aligned}
 \text{ABC}^{\text{ve}}(G) &= \sum_{uv \in E(G)} \sqrt{\frac{\Lambda_{ve}(u) + \Lambda_{ve}(v) - 2}{(\Lambda_{ve}(u)\Lambda_{ve}(v))}}, \\
 \text{ABC}^{\text{ve}}(G) &= \left(\sqrt{\frac{5}{10}}\right)|E_1^*| + \left(\sqrt{\frac{8}{24}}\right)|E_2^*| + \left(\sqrt{\frac{11}{40}}\right)|E_3^*| \\
 &\quad + \left(\sqrt{\frac{12}{48}}\right)|E_4^*| + \left(\sqrt{\frac{14}{64}}\right)|E_5^*| \\
 &= \left(\sqrt{\frac{5}{10}}\right)(4p + 4q + 4r - 8) + \left(\sqrt{\frac{8}{24}}\right) \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + \left(\sqrt{\frac{11}{40}}\right)(4p + 4q + 4r - 8) + \left(\sqrt{\frac{12}{48}}\right) \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + \left(\sqrt{\frac{14}{64}}\right)[8(q - 1)(p - 1)(r - 1)] \\
 &= \left(\frac{4}{\sqrt{2}} - \frac{4}{\sqrt{3}} + 2\sqrt{\frac{11}{10}}\right)[q + p + r] \\
 &\quad + \left(\frac{2}{\sqrt{3}} + 1 - \sqrt{14}\right)[pq + qr + pr] \\
 &\quad + \sqrt{14}pqr + \left(2\sqrt{3} + \sqrt{14} + 7 - 4\sqrt{\frac{11}{10}}\right).
 \end{aligned}$$

(d) The geometric-arithmetic index:

$$\begin{aligned}
 \text{GA}^{\text{ve}}(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{\Lambda_{ve}(u) \times \Lambda_{ve}(v)}}{(\Lambda_{ve}(u) + \Lambda_{ve}(v))}, \\
 \text{GA}^{\text{ve}}(G) &= \left(\frac{2\sqrt{10}}{7}\right)|E_1^*| + \left(\frac{2\sqrt{24}}{10}\right)|E_2^*| + \left(\frac{2\sqrt{40}}{13}\right)|E_3^*| \\
 &\quad + \left(\frac{2\sqrt{48}}{14}\right)|E_4^*| + \left(\frac{2\sqrt{64}}{16}\right)|E_5^*| \\
 &= \left(\frac{2\sqrt{10}}{7}\right)(4p + 4q + 4r - 8) + \left(\frac{2\sqrt{24}}{10}\right) \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + \left(\frac{2\sqrt{40}}{13}\right)(4p + 4q + 4r - 8) + \left(\frac{2\sqrt{48}}{14}\right) \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + \left(\frac{2\sqrt{64}}{16}\right)[8(q - 1)(p - 1)(r - 1)] \\
 &= 8\left(\frac{\sqrt{10}}{7} + \frac{\sqrt{6}}{5} + \frac{2\sqrt{10}}{13} + \frac{2\sqrt{3}}{7} + 1\right) \\
 &\quad \times [q + p + r] + 4\left(\frac{\sqrt{6}}{5} + \frac{2\sqrt{3}}{7} + 2\right) \\
 &\quad \times [pq + qr + pr] + 8pqr \\
 &\quad + \left(8 + \frac{12\sqrt{6}}{5} - \frac{16\sqrt{10}}{7} - \frac{32\sqrt{10}}{13} + \frac{24\sqrt{3}}{7}\right).
 \end{aligned}$$

(a)

(b)

Figure 5: (a) The first Zagreb β -index(I) and (b) the second Zagreb index.

Figure 6: (a) The atom-bond connectivity index and (b) the geometric-arithmetic index.

(e) The Harmonic index:

$$\begin{aligned}
 H^{ve}(G) &= \sum_{uv \in E(G)} \frac{2}{\Lambda_{ve}(u) + \Lambda_{ve}(v)}, \\
 H^{ve}(G) &= \left(\frac{2}{7}\right)|E_1^*| + \left(\frac{2}{10}\right)|E_2^*| + \left(\frac{2}{13}\right)|E_3^*| \\
 &\quad + \left(\frac{2}{14}\right)|E_4^*| + \frac{2}{14}|E_5^*| \\
 &= \left(\frac{2}{7}\right)(4p + 4q + 4r - 8) + \left(\frac{2}{10}\right)(2pq + 2pr \\
 &\quad + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + \left(\frac{2}{13}\right)(4p + 4q + 4r - 8) + \left(\frac{2}{14}\right) \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + \frac{2}{14}[8(q - 1)(p - 1)(r - 1)] \\
 &= \frac{631}{455}(q + p + r) + \frac{59}{35}(pq + qr + pr) \\
 &\quad + pqr + \frac{209}{455}.
 \end{aligned}$$

(f) The sum-connectivity index:

$$\begin{aligned}
 \chi^{ve}(G) &= \sum_{uv \in E(G)} (\Lambda_{ve}(u) + \Lambda_{ve}(v))^{-\frac{1}{2}}, \\
 \chi^{ve}(G) &= (7)^{-\frac{1}{2}}|E_1^*| + (10)^{-\frac{1}{2}}|E_2^*| + (13)^{-\frac{1}{2}}|E_3^*| \\
 &\quad + (14)^{-\frac{1}{2}}|E_4^*| + (16)^{-\frac{1}{2}}|E_5^*| \\
 &= (7)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (10)^{-\frac{1}{2}}(2pq + 2pr \\
 &\quad + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + (13)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (14)^{-\frac{1}{2}}(2pq \\
 &\quad + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + (16)^{-\frac{1}{2}}[8(q - 1)(p - 1)(r - 1)] \\
 &= 4\left(\frac{1}{\sqrt{7}} - \frac{1}{\sqrt{10}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{14}} + 1\right)[q + p + r] \\
 &\quad + \left(\frac{2}{\sqrt{10}} + \frac{2}{\sqrt{14}} + 4\right)[pq + qr + pr] \\
 &\quad + 4pqr + \left(\frac{6}{\sqrt{10}} - \frac{8}{\sqrt{7}} - \frac{8}{\sqrt{13}} + \frac{6}{\sqrt{14}} + 4\right).
 \end{aligned}$$

Figure 7: (a) The Harmonic index and (b) the sum-connectivity index.

Figure 8: The andic index.

(g) The Randic index:

$$\begin{aligned}
 R^{ve}(G) &= \sum_{uv \in E(G)} (\Lambda_{ve}(u) \Lambda_{ve}(v))^{-\frac{1}{2}}, \\
 R^{ve}(G) &= (10)^{-\frac{1}{2}} |E_1^*| + (24)^{-\frac{1}{2}} |E_2^*| + (40)^{-\frac{1}{2}} |E_3^*| \\
 &\quad + (48)^{-\frac{1}{2}} |E_4^*| + (64)^{-\frac{1}{2}} |E_5^*| \\
 &= (10)^{-\frac{1}{2}} (4p + 4q + 4r - 8) + (24)^{-\frac{1}{2}} \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + (40)^{-\frac{1}{2}} (4p + 4q + 4r - 8) + (48)^{-\frac{1}{2}} \\
 &\quad \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \\
 &\quad + (64)^{-\frac{1}{2}} [8(q-1)(p-1)(r-1)] \\
 &= \left(\frac{6}{\sqrt{10}} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}} + 1 \right) [q + p + r] \\
 &\quad + \left(\frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{3}} - 1 \right) [pq + qr + pr] \\
 &\quad + pqr + \left(\frac{-12}{\sqrt{10}} + \frac{3}{\sqrt{6}} - \frac{\sqrt{3}}{2} - 1 \right).
 \end{aligned}$$

5 Numerical results and discussion for $\text{Cu}_2\text{O}(G)$

We present mathematical outcomes identified with the ev-degree- and ve-degree-based topological descriptors for the cuprite oxide sub-atomic structures. We have utilized multiple estimations of p , q , and r , which have figured mathematical tables, and drawn the graph 3–8 for the cuprite oxide sub-atomic structure to analyze the conduct of above-processed topological descriptors. (Tables 4 and 5).

The Zagreb-types indices were computed for the complete π -electron energy of atoms, and energy is expanding request for the instance of the copper oxide for higher estimations of p , q , and r [26].

The Randic record can be utilized for substance comparability of sub-atomic mixes and in figuring the Kovats constants and limit of particles, and empower in programme dynamic. Randic lists the copper oxide extensions with the expansion in p , q , and r [27].

It has been observed that the prescient intensity of the mathematical number-crunching record is better than contrasted and the Randic availability file. GA record for the copper oxide increments with the augmentation in p , q , and r .

The molecule bond network (ABC) record gives an acceptable connection to figure out the strain energy of cycloalkanes just as for the security of straight and spread alkanes [28]. The ABC file for the copper oxide increments with p , q , and r . In the current work, ABC file increases for the copper oxide with the increase of p , q , and r .

Table 4: Numerical representation of the computed indices for certain values of Cu_2O

$[p, q, r]$	$M^{ev}(\text{Cu}_2\text{O})$	$M_1^{ave}(\text{Cu}_2\text{O})$	$M_1^{bve}(\text{Cu}_2\text{O})$	$M_2^{bve}(\text{Cu}_2\text{O})$	$R^{ve}(\text{Cu}_2\text{O})$
[1, 1, 1]	628	180	80	2288	1.8974
[2, 2, 2]	3328	1824	592	8248	15.8764
[3, 3, 3]	9708	7212	2160	21088	43.5011
[4, 4, 4]	21496	18648	5552	43880	90.7714
[5, 5, 5]	40420	38436	11536	79696	163.6873
[6, 6, 6]	68208	68880	20880	131608	268.2489
[7, 7, 7]	106588	112284	34352	202688	410.4561
[8, 8, 8]	157288	170952	52720	296008	596.309
[9, 9, 9]	222036	247188	76752	414640	831.8075
[10, 10, 10]	302560	343296	107216	561656	1122.952

Table 5: Numerical representation of the computed indices for certain values of Cu_2O

$[p, q, r]$	$R^{\text{ev}}(\text{Cu}_2\text{O})$	$ABC^{\text{ve}}(\text{Cu}_2\text{O})$	$GA^{\text{ve}}(\text{Cu}_2\text{O})$	$H^{\text{ve}}(\text{Cu}_2\text{O})$	$\chi^{\text{ve}}(\text{Cu}_2\text{O})$
[1, 1, 1]	2.0097	14.5318	118.7754	10.6769	41.0356
[2, 2, 2]	11.4733	34.2908	352.3796	37.0088	134.8145
[3, 3, 3]	33.1389	89.4278	753.6179	85.4549	307.5953
[4, 4, 4]	75.0066	202.393	1370.491	162.0154	583.3779
[5, 5, 5]	145.0763	395.6362	2250.999	272.6901	986.1628
[6, 6, 6]	251.348	691.6074	3443.142	423.4791	1539.9491
[7, 7, 7]	401.8218	1112.756	4994.918	620.3824	2268.7373
[8, 8, 8]	604.4976	1681.5339	6954.33	869.4	3196.5276
[9, 9, 9]	867.3755	2420.388	9369.375	1176.532	4347.3196
[10, 10, 10]	1198.455	3351.7704	12288.06	1547.778	5745.1136

6 Conclusion

Topological indices methodology has opened up a broad variety of possible applications for the QSAR estimation of antiparasitic drugs and many others. It is important to understand the graphs and networks underlying topologies through topological descriptors. These experimental studies have a broad range of applications in the fields of chem-informatics, bio-medicine- and bio-informatics, where various graph topological-based assessments are used to tackle many complicated schemes. This topological study may help in the electronic and atomic structure of oxygen-dosed and clean of Cu_2O single-crystal surfaces, and all new experimental information may concern the defect structure in non-stoichiometric Cu_2O . In future, we are interested in calculating the neighborhood M-polynomial for the chemical structure of Cu_2O .

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