Research Article

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On ve-degree- and ev-degree-based topological properties of crystallographic structure of cuprite \( \text{Cu}_2\text{O} \)

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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 \( (\text{Cu}_2\text{O}) \) 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 \( \text{Cu}_2\text{O} \)

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].
The Randic index is by far the most prominent, most frequently used and studied topological index of all others. Gutman and Trinajstic 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 ($M^e$) index and Randic ($R^e$) index for any edge $e = uv \in E(G)$ are defined as

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

**ve-degree-based indices**

For a connected graph $G$, the ve-degree-based first Zagreb alpha ($M^v_{1}$) index and second Zagreb ($M^v_{2}$) index for any vertex $v \in V(G)$ is defined as

$$M^v_{1}(G) = \sum_{v \in V} \Lambda_{ve}(v)^2.$$

**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 ($M^v_{1}$) index, second Zagreb ($M^v_{2}$) index, atom-bond connectivity (ABC$^v$) index, geometric-arithmetic ($GA^v$) index, Harmonic ($H^v$) index, sum-connectivity ($\chi^v$) index, and the Randic ($R^v$) index for each edge $uv \in E(G)$ are defined as

$$M^v_{1}(G) = \sum_{uv \in E} \Lambda_{ve}(u) + \Lambda_{ve}(v),$$

$$M^v_{2}(G) = \sum_{uv \in E} \Lambda_{ve}(u) \times \Lambda_{ve}(v),$$

$$ABC^v(G) = \sum_{uv \in E} \sqrt{\frac{\Lambda_{ve}(u) + \Lambda_{ve}(v) - 2}{\Lambda_{ve}(u) \times \Lambda_{ve}(v)}},$$

$$GA^v(G) = \sum_{uv \in E} \frac{2\Lambda_{ve}(u) \times \Lambda_{ve}(v)}{\Lambda_{ve}(u) + \Lambda_{ve}(v)},$$

$$H^v(G) = \sum_{uv \in E} \frac{2}{\Lambda_{ve}(u) + \Lambda_{ve}(v)},$$

$$\chi^v(G) = \sum_{uv \in E} (\Lambda_{ve}(u) + \Lambda_{ve}(v))^2,$$

$$R^v(G) = \sum_{uv \in E} (\Lambda_{ve}(u) \times \Lambda_{ve}(v))^2.$$

2 **Methodology**

Mathematica was used for computing results for ev-degree, ve-degree, and end 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$_2$O)**

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$_2$O) is a commonly occurred copper corrosion product, and new applications of Cu$_2$O 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
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 transport 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; CuO²⁻ have attracted considerable attention among various transition metal oxides in recent years [22]. Today, CuO²⁻’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 CuO²⁻, which is a crystallographic structure, see data in [24,25]. Copper oxide (CuO) primary highlights where Cu are copper and O are oxygen iotas. The CuO²⁻ grid is shaped by interpenetrating the Cu and O molecules, see Figure 1a. Unit cell of CuO²⁻ 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 CuO²⁻ grid, each CuO²⁻ particle is composed of two O iotas, and every O molecule is facilitated with four Cu iotas.

The CuO²⁻ lattice developed in the p × q plane and accumulated it in r layers, see Figure 2. The crystal structure of CuO²⁻ contains the 1 + p + q + pq + r + pr + qr + 6pq r vertices and 8pq r edges, respectively. On the base of degrees, the vertices of CuO²⁻ 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 two, and 2pq r − pq − pr + q + p + r − 1 vertices of degree four. Similarly, the edges of CuO²⁻ are partitioned as E₁; 2 with 4(p + q + r − 2) edges, E₂; 2, with 2(pq + pr + qr − 2p − 2q − 2r + 3) edges, and E₃; 4 having 8pq r − 4pq − 4pr − 4qr + 4p + 4q + 4r − 4.

4 Main results

Theorem 1. Let G be a molecular graph of cuprite CuO²⁻, then ev-degree-based Zagreb index and ev-degree-based Randic index are given by,

Figure 1: (a) Copper oxide (CuO²⁻) structural features where Cu are copper and O are oxygen atoms and (b) unit cell of copper oxide (CuO²⁻) lattice.

Figure 2: (a) Unit cell of CuO²⁻[1, 1, 1] and (b) the crystallographic structure of CuO²⁻[3, 2, 3].
(a) $M^{ev}(G) = 116(p + q + r) - 112(pq + pr - qr) + 288pqr - 120$

(b) $R^{ev}(G) = \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)p + \left(\frac{4}{\sqrt{3}} - 2 + \frac{4}{\sqrt{6}}\right)q$

Proof. From the structure of Cu$_2$O, we divide the vertices into three partitions $E_{1,2}$, $E_{2,3}$ 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.

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

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

$M^{ev}(G) = \sum_{ee \in E(G)} \Lambda_{ev}(e)^2$, 

$M^{ev}(G) = (3)^{\frac{1}{2}}|E_{1,2}| + (4)^{\frac{1}{2}}|E_{2,3}| + (6)^{\frac{1}{2}}|E_{2,4}|

= 9(4p + 4q + 4r - 8) + 16(2pq + 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.

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

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

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

= (3)^{\frac{1}{2}}(4p + 4q + 4r - 8) + (4)^{\frac{1}{2}}(2pq + 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

+ \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).

Table 2: The vertices ev-degrees of Cu$_2$O

<table>
<thead>
<tr>
<th>$N(u)$</th>
<th>$\Lambda_{ev}(u)$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>4(p + q + r - 2)</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>2pq + 2qr + qr - 2p - 2q - 2r + 3</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>4q + 4p + 4r - 8</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>4pq + 4qr - 4p - 4q + 4r - 12</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>4qr - 4qr - 4q + 4r</td>
</tr>
<tr>
<td>4</td>
<td>8</td>
<td>2pqr - pq - qr - pr + q + p + r - 1</td>
</tr>
</tbody>
</table>

Theorem 2. Let $G$ be a molecular graph of cuprite Cu$_2$O, then vertices ev-degree-based first Zagreb a-index is given by,

$M^1_{ev}(G) = 84(p + q + r) - 144(pq + pr + qr) + 384pqr - 24$

Proof. From the structure of Cu$_2$O, 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 ev-degrees, we have calculated the vertices ev-degrees as shown in Table 2.

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

$M^1_{ev}(G) = \sum_{u \in V(G)} \Lambda_{ev}(v)^2$, 

$M^1_{ev}(G) = (0)^2(4) + (2)^2(4p + 4q + 4r - 8)$

+ (4)^2(2pq + 2pr + 2qr - 4p - 4q - 4r + 6) + (5)^2(4p + 4q + 4r - 8) + (6)^2(4q + 4qr$ + 4q r - 4q - 4r - 12$)

+ (8)^2[4(q - 1)(p - 1)(r - 1)] + (8)^2(2pqr - pq - qr - pr + q + p + r - 1)$

= 84(q + p + r) - 144(pq + qr + pr) + 384pqr - 24.$

Theorem 3. Let $G$ be a molecular graph of cuprite Cu$_2$O, then end vertices ev-degree-based indices of each edges are given by,

(a) $M^1_{ev}(G) = 112(q + p + r) - 80(pq + qr + pr)$

+ 128pqr - 144

(b) $M^2_{ev}(G) = 424(q + p + r) - 368(pq - qr - pr)$

+ 512pqr + 136

Table 1: The edges ev-degree of Cu$_2$O

<table>
<thead>
<tr>
<th>$(A(u), N(v))$</th>
<th>$\Lambda_{ev}(e)$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>E$_{1,2}$</td>
<td>3</td>
<td>4p + 4q + 4r - 8</td>
</tr>
<tr>
<td>E$_{2,3}$</td>
<td>4</td>
<td>2(pq + pr + qr - 2p - 2q - 2r + 3)</td>
</tr>
<tr>
<td>E$_{2,4}$</td>
<td>6</td>
<td>8pqr - 4pq - 4pr - 4qr + 4p + 4q + 4r - 4</td>
</tr>
</tbody>
</table>
(c) $\text{ABC}^{ve}(G) = \left( \frac{4}{\sqrt{3}} - \frac{4}{\sqrt{7}} + 2\frac{\sqrt{11}}{10} \right) [p + q + r]$
\[+ \left( \frac{2}{\sqrt{3}} + 1 - \sqrt{4} \right) [pq + pr + qr] \]
\[+ \sqrt{4} pq + \left( 2\frac{\sqrt{3}}{7} + \sqrt{14} + 7 - 4\frac{\sqrt{11}}{10} \right) \]

(d) $\text{GAE}^{ve}(G) = 8 \left( \frac{\sqrt{10}}{7} + \frac{\sqrt{6}}{5} + \frac{2\sqrt{10}}{13} + \frac{2\sqrt{3}}{7} + 1 \right) [p + q + r]$
\[+ 4 \left( \frac{\sqrt{6}}{5} + 2\frac{\sqrt{3}}{7} + 2 \right) [pq + pr + qr] + 8pq + qr \]
\[+ \left( 8 + \frac{12\sqrt{6}}{5} - \frac{16\sqrt{10}}{7} - \frac{32\sqrt{6}}{13} + \frac{24\sqrt{3}}{7} \right) \]

(e) $\text{H}^{ve}(G) = \frac{631}{455}(p + q + r) + \frac{59}{35}(pq + pr + qr) + pqr + \frac{209}{555}$

(f) $\chi^{ve}(G) = 4 \left( \frac{1}{\sqrt{7}} - \frac{1}{\sqrt{10}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{14}} + 1 \right) [p + q + r]$
\[+ \left( \frac{2}{\sqrt{10}} + \frac{2}{\sqrt{6}} + 4 \right) [pq + pr + qr] + 4pq + qr \]
\[+ \left( \frac{6}{\sqrt{10}} - \frac{8}{\sqrt{7}} - \frac{8}{\sqrt{13}} + \frac{6}{\sqrt{4}} + 4 \right) \]

(g) $R^{ve}(G) = \left( \frac{6}{\sqrt{10}} - \frac{2}{\sqrt{5}} - \frac{1}{\sqrt{3}} + 1 \right) [p + q + r]$
\[+ \left( \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} - 1 \right) [pq + pr + qr] + pqr \]
\[+ \left( \frac{12}{\sqrt{10}} + \frac{3}{\sqrt{6}} - \frac{\sqrt{3}}{2} - 1 \right) \]

**Proof.** From the structure of Cu$_2$O, we divide the edges into three partitions $E_{1,2}, E_{2,3},$ 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.

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 $\beta$-index:

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

\[M_2^{\text{ev}}(G) = \sum_{uv \in E(G)} (\Lambda_{ve}(u) + \Lambda_{ve}(v)) \]

\[= (7)(4p + 4q + 4r - 8) + (10)(2pq + 2pr + 2qr - 4p - 4q - 4r + 12) + (13)(4p + 4q + 4r - 8) + (14)(2pq + 2pr + 2qr - 4p - 4q - 4r + 12) + (16)(8q - 8) + 80(pq +qr + pr) + 128pq + 144r \]

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

**Figure 4:** The first Zagreb $\alpha$-index.
The atom-bond connectivity index:

\[ \sum() = (\Lambda_{uv}(u) + \Lambda_{uv}(v) - 2)/\Lambda_{uv}(u)\Lambda_{uv}(v) \]

\[ \Lambda^{A_{uv}}(G) = \sum_{uv \in E(G)} \left[ (5/10)E_1^1 + (8/24)E_2^1 + (11/40)E_3^1 \right. \\
+ \left. (12/48)E_4^1 + (14/64)E_5^1 \right] \\
= \left( \frac{5}{10} \right)(4p + 4q + 4r - 8) + \left( \frac{8}{24} \right)(2pq + 2pr + 2qr - 4q - 4r + 12) \\
+ \left( \frac{11}{40} \right)(4p + 4q + 4r - 8) + \left( \frac{12}{48} \right)(2pq + 2pr + 2qr - 4q - 4r + 12) \\
+ \left( \frac{14}{64} \right)(8q - 1)(p - 1)(r - 1)] \\
= \left( \frac{4}{\sqrt{2}} - \frac{4}{\sqrt{3}} + 2\sqrt{10} \right)[q + p + r] \\
+ \left( \frac{2}{\sqrt{3}} + 1 - \sqrt{10} \right)[pq + qr + pr] \\
+ \sqrt{14}pq + \left( 2\sqrt{3} + \sqrt{14} + 7 - 4\sqrt{10} \right).

(c) The atom-bond connectivity index:

\[ \Lambda^{A_{uv}}(G) = \sum_{uv \in E(G)} \left( \Lambda_{uv}(u) + \Lambda_{uv}(v) - 2 \right)/\Lambda_{uv}(u)\Lambda_{uv}(v) \]

\[ \Lambda^{A_{uv}}(G) = \left( \frac{5}{10} \right)[E_1^1] + \left( \frac{8}{24} \right)[E_2^1] + \left( \frac{11}{40} \right)[E_3^1] \\
+ \left( \frac{12}{48} \right)[E_4^1] + \left( \frac{14}{64} \right)[E_5^1] \\
= \left( \frac{5}{10} \right)(4p + 4q + 4r - 8) + \left( \frac{8}{24} \right)(2pq + 2pr + 2qr - 4q - 4r + 12) \\
+ \left( \frac{11}{40} \right)(4p + 4q + 4r - 8) + \left( \frac{12}{48} \right)(2pq + 2pr + 2qr - 4q - 4r + 12) \\
+ \left( \frac{14}{64} \right)(8q - 1)(p - 1)(r - 1)] \\
= \left( \frac{4}{\sqrt{2}} - \frac{4}{\sqrt{3}} + 2\sqrt{10} \right)[q + p + r] \\
+ \left( \frac{2}{\sqrt{3}} + 1 - \sqrt{10} \right)[pq + qr + pr] \\
+ \sqrt{14}pq + \left( 2\sqrt{3} + \sqrt{14} + 7 - 4\sqrt{10} \right).

(d) The geometric-arithmetic index:

\[ \Lambda^{G_{uv}}(G) = \sum_{uv \in E(G)} \left( \Lambda_{uv}(u) + \Lambda_{uv}(v) - 2 \right)/\Lambda_{uv}(u)\Lambda_{uv}(v) \]

\[ \Lambda^{G_{uv}}(G) = \left( \frac{5}{10} \right)[E_1^1] + \left( \frac{8}{24} \right)[E_2^1] + \left( \frac{11}{40} \right)[E_3^1] \\
+ \left( \frac{12}{48} \right)[E_4^1] + \left( \frac{14}{64} \right)[E_5^1] \\
= \left( \frac{5}{10} \right)(4p + 4q + 4r - 8) + \left( \frac{8}{24} \right)(2pq + 2pr + 2qr - 4q - 4r + 12) \\
+ \left( \frac{11}{40} \right)(4p + 4q + 4r - 8) + \left( \frac{12}{48} \right)(2pq + 2pr + 2qr - 4q - 4r + 12) \\
+ \left( \frac{14}{64} \right)(8q - 1)(p - 1)(r - 1)] \\
= \left( \frac{4}{\sqrt{2}} - \frac{4}{\sqrt{3}} + 2\sqrt{10} \right)[q + p + r] \\
+ \left( \frac{2}{\sqrt{3}} + 1 - \sqrt{10} \right)[pq + qr + pr] \\
+ \sqrt{14}pq + \left( 2\sqrt{3} + \sqrt{14} + 7 - 4\sqrt{10} \right).

Table 3: Ve-degrees of end vertices of each edge of Cu2O

<table>
<thead>
<tr>
<th>Edge</th>
<th>(Anv(u), Anv(v))</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>E_1^1</td>
<td>(2, 5)</td>
<td>4p + 4q + 4r - 8</td>
</tr>
<tr>
<td>E_2^1</td>
<td>(4, 6)</td>
<td>2pq + 2pr + 2qr - 4q - 4r + 12</td>
</tr>
<tr>
<td>E_3^1</td>
<td>(5, 8)</td>
<td>4(p + q + r - 2)</td>
</tr>
<tr>
<td>E_4^1</td>
<td>(6, 8)</td>
<td>2pq + 2pr + 2qr - 4q - 4r + 12</td>
</tr>
<tr>
<td>E_5^1</td>
<td>(8, 8)</td>
<td>8(q - 1)(p - 1)(r - 1)</td>
</tr>
</tbody>
</table>

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

\[ H^{ve}(G) = \sum_{uv \in E(G)} \frac{2}{\Lambda_{uv}(u) + \Lambda_{uv}(v)}. \]

\[ H^{ve}(G) = \left( \frac{2}{7} |E_1| + \frac{2}{10} |E_2| + \frac{2}{13} |E_3| \right) \]

\[ + \left( \frac{2}{14} |E_4| + \frac{2}{14} |E_5| \right) \]

\[ = \left( \frac{2}{7} (4p + 4q + 4r - 8) + \frac{2}{10} (2pq + 2pr \right. \]

\[ + 2qr - 4p - 4q - 4r + 12 \]

\[ + \frac{2}{13} (4p + 4q + 4r - 8) + \frac{2}{14} \right) \]

\[ \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \]

\[ + \frac{2}{14} [8(q - 1)(p - 1)(r - 1)] \]

\[ = \frac{631}{455} (q + p + r) + \frac{59}{35} (pq + qr + pr) \]

\[ + pqr + \frac{209}{455}. \]

The sum-connectivity index:

\[ \chi^{ve}(G) = \sum_{uv \in E(G)} \left( \Lambda_{uv}(u) + \Lambda_{uv}(v) \right)^{-\frac{1}{2}}, \]

\[ \chi^{ve}(G) = (7)^{-\frac{1}{2}}|E_1| + (10)^{-\frac{1}{2}}|E_2| + (13)^{-\frac{1}{2}}|E_3| \]

\[ + (14)^{-\frac{1}{2}}|E_4| + (16)^{-\frac{1}{2}}|E_5| \]

\[ = (7)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (10)^{-\frac{1}{2}}(2pq + 2pr \]

\[ + 2qr - 4p - 4q - 4r + 12 \]

\[ + (13)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (14)^{-\frac{1}{2}}(2pq \]

\[ + 2pr + 2qr - 4p - 4q - 4r + 12 + (16)^{-\frac{1}{2}}[8(q - 1)(p - 1)(r - 1)] \]

\[ = 4 \left( \frac{1}{\sqrt{7}} - \frac{1}{\sqrt{10}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{14}} + 1 \right) [q + p + r] \]

\[ + \left( \frac{2}{\sqrt{10}} + \frac{2}{\sqrt{14}} + 4 \right) [pq + qr + pr] \]

\[ + 4pqr + \left( \frac{6}{\sqrt{10}} - \frac{8}{\sqrt{13}} - \frac{8}{\sqrt{14}} + \frac{6}{\sqrt{14}} + 4 \right). \]
The Randic index:

\[ R^{\text{ev}}(G) = \sum_{uv \in E(G)} (\Lambda_{\text{ev}}(u) \Lambda_{\text{ev}}(v))^{-\frac{1}{2}}, \]

\[ R^{\text{ev}}(G) = (10)^{-\frac{1}{2}}[E_v^1] + (24)^{-\frac{1}{2}}[E_v^2] + (40)^{-\frac{1}{2}}[E_v^3] \]
\[ + (48)^{-\frac{1}{2}}[E_v^4] + (64)^{-\frac{1}{2}}[E_v^5] \]
\[ = (10)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (24)^{-\frac{1}{2}} \]
\[ \times (2pq + 2pr + 2qr - 4p - 4q - 4r + 12) \]
\[ + (40)^{-\frac{1}{2}}(4p + 4q + 4r - 8) + (48)^{-\frac{1}{2}} \]
\[ \times (2pq + 2pr + 2qr - 4p - 4q - 4r - 8) + (64)^{-\frac{1}{2}}[8(q - 1)(p - 1)(r - 1)] \]
\[ = \left( \frac{6}{\sqrt{10}} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}} + 1 \right)[q + p + r] \]
\[ + \left( \frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{3}} - \frac{1}{2} \right)pq + qr + pr \]
\[ + pq + \left( -\frac{12}{\sqrt{10}} + \frac{3}{\sqrt{6}} - \frac{\sqrt{3}}{2} - 1 \right). \]

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 \( \pi \)-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 \( \text{Cu}_2\text{O} \)

<table>
<thead>
<tr>
<th>([p, q, r])</th>
<th>(M^{\text{ev}}(\text{Cu}_2\text{O}))</th>
<th>(M^{\text{ve}}_{1}(\text{Cu}_2\text{O}))</th>
<th>(M^{\text{ve}}_{2}(\text{Cu}_2\text{O}))</th>
<th>(R^{\text{ev}}(\text{Cu}_2\text{O}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>[1, 1, 1]</td>
<td>628</td>
<td>180</td>
<td>80</td>
<td>2288</td>
</tr>
<tr>
<td>[2, 2, 2]</td>
<td>3328</td>
<td>1824</td>
<td>592</td>
<td>8248</td>
</tr>
<tr>
<td>[3, 3, 3]</td>
<td>9708</td>
<td>7212</td>
<td>2160</td>
<td>21088</td>
</tr>
<tr>
<td>[4, 4, 4]</td>
<td>21496</td>
<td>18648</td>
<td>5552</td>
<td>43880</td>
</tr>
<tr>
<td>[5, 5, 5]</td>
<td>68208</td>
<td>68880</td>
<td>11536</td>
<td>79696</td>
</tr>
<tr>
<td>[6, 6, 6]</td>
<td>106588</td>
<td>112284</td>
<td>20880</td>
<td>131608</td>
</tr>
<tr>
<td>[7, 7, 7]</td>
<td>157288</td>
<td>170952</td>
<td>34352</td>
<td>202688</td>
</tr>
<tr>
<td>[8, 8, 8]</td>
<td>122036</td>
<td>247188</td>
<td>252720</td>
<td>296008</td>
</tr>
<tr>
<td>[9, 9, 9]</td>
<td>302560</td>
<td>343296</td>
<td>107216</td>
<td>561656</td>
</tr>
<tr>
<td>[10, 10, 10]</td>
<td>302560</td>
<td>343296</td>
<td>107216</td>
<td>561656</td>
</tr>
</tbody>
</table>
Table 5: Numerical representation of the computed indices for certain values of Cu₂O

<table>
<thead>
<tr>
<th>[p, q, r]</th>
<th>R²m(Cu₂O)</th>
<th>ABC²m(Cu₂O)</th>
<th>GA²m(Cu₂O)</th>
<th>H²m(Cu₂O)</th>
<th>Χ²m(Cu₂O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[1, 1, 1]</td>
<td>2.0097</td>
<td>14.5318</td>
<td>118.7754</td>
<td>10.6769</td>
<td>41.0356</td>
</tr>
<tr>
<td>[2, 2, 2]</td>
<td>11.4733</td>
<td>34.2908</td>
<td>352.3796</td>
<td>37.0088</td>
<td>134.8145</td>
</tr>
<tr>
<td>[3, 3, 3]</td>
<td>33.1389</td>
<td>89.4278</td>
<td>753.6179</td>
<td>85.4549</td>
<td>307.5953</td>
</tr>
<tr>
<td>[4, 4, 4]</td>
<td>75.0066</td>
<td>202.393</td>
<td>1370.491</td>
<td>162.0154</td>
<td>583.3779</td>
</tr>
<tr>
<td>[6, 6, 6]</td>
<td>251.348</td>
<td>691.6074</td>
<td>3443.142</td>
<td>423.4791</td>
<td>1539.9491</td>
</tr>
<tr>
<td>[7, 7, 7]</td>
<td>401.8218</td>
<td>1112.756</td>
<td>4994.918</td>
<td>620.3824</td>
<td>2268.7373</td>
</tr>
<tr>
<td>[8, 8, 8]</td>
<td>604.4976</td>
<td>1681.5339</td>
<td>7545.1136</td>
<td>869.4</td>
<td>3196.5276</td>
</tr>
<tr>
<td>[9, 9, 9]</td>
<td>867.3755</td>
<td>2420.388</td>
<td>9369.375</td>
<td>1176.532</td>
<td>4347.3196</td>
</tr>
<tr>
<td>[10, 10, 10]</td>
<td>1198.455</td>
<td>3351.7704</td>
<td>12288.06</td>
<td>1547.778</td>
<td>5745.1136</td>
</tr>
</tbody>
</table>

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 Cu₂O single-crystal surfaces, and all new experimental information may concern the defect structure in non-stoichiometric Cu₂O. In future, we are interested in calculating the neighborhood M-polynomial for the chemical structure of Cu₂O.

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References


