Section A-Research paper
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copper(I) oxide molecular descriptors based on `$ve$ degree and `ev degree

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Abstract. Copper oxide is a well-known inorganic chemical and p-type semiconductor. It's a chemical element with the formula Cu_2O and it's employed in chemical sensors and solar cells. The results of various ι degree based and κ degree based topological indices of Cu_2O were found in this study. Throughout the article we denote `ve = ι and `ev = κ. In addition, the maple was used to plot these research discoveries.
Keywords: Copper(I) Oxide, polynomial, topological index, M-polynomial, crystallographic structure.
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1 Introduction

One of the key reasons for the expansion is the ability to quickly examine quantitative structure-property or quantitative structure activity relationships (QSPR/QSAR). In a chemical plot, the vertex grade is frequently indicated for its valence. Graph theory has been a focal point for the development of many modern scientific principles and their application to several fields of chemistry. Copper oxide has non-toxic qualities, is complete, and is easy to assemble. Chemists can think as much as they want about molecules and their chemical behaviour by looking at their molecularplot aspects, thanks to the advent of the topological theory of chemistry. Chemical graph theory is a field of mathematics that uses graph theory to analyze the molecular structure of chemical compounds. The topological index is a part of chemical graph theory that connects the physicochemical properties of the underlying chemical graphs, such as viscosity, density, infrared spectrum, boiling point, and melting point. A large number of works on topological indices are available to the reader. [3], [12], [13], [14], [15], [11].

Copper (I) oxide is used in marine paints as a pigment, fungicide, and anti-fouling agent, among other things. Copper (II) oxide is an important product that serves as a starting point for the synthesis of additional copper salts. It has a variety of uses, including wood preservatives, coloured glazes in ceramics, animal feed additives, and welding using copper alloys and other materials.

Photochemical effects, stability, pigment, fungicide, non-toxicity, and low cost are all major benefits. It can be used in a variety of disciplines, including new energy, sensing, sterilising, and others. Understanding cuprite at the electrical and atomic level is more helpful in predicting and controlling the processes of copper corrosion.

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In this study, we calculated the polynomials of both κ and ι degree topological indices for the chemical structure of copper oxide, and explored a few early ideas of both ι degree and κ degree. Additionally, the ability of these trials to address a wide range of complex methods is illustrated in the fields of chem-informatics, bio-medicine, and bio-informatics, where graph topological assessments are regularly employed to further develop and understand the mathematical aspects of the real-world network model.

Using vertex-edge domination and edge-vertex domination parameters, Chellali and his colleagues [2] have published a research paper. In graph theory, they defined κ degrees and ι degrees, which are two novel degree graph invariants. As a result, they discovered that the total κ and ι degrees for any graph are closely linked to the first Zagreb index, a prominent degee-based topological index. In this paper, we computed various topological indices such as the K-index, Sombar index, VL-index, Nirmala index, and Albertson index, all of which are based on κ and ι degrees.

The Wiener index, also referred to as the path number, was the first index name and was introduced by Wiener in 1965 along with the topological descriptor. Ten years later, Randic proposed the Randic-type index, a topological index. The Randic index is still the most well-known, commonly used, and studied of all the topological indices that have since been created. However, the majority of research projects used the traditional concept of degrees, such as Randic and Zagreb indices. This work translated the classical notion of degrees into κ and ι degrees for recently introduced topological indices, such as the K-index, VL-index, Nirmala index, Albertson index, and Sombor index.

Let Ψ be a graph with vertices α and β, $\Psi = (\alpha, \beta)$ use this notation throughout the article. Since degree-based topological indices may be used to analyze the chemical characteristics of various molecule structures, they are helpful. We are particularly interested in polynomial-based topological indices as a result of this inspiration. Topological indices based on polynomials are a useful method for predicting a compound's physicochemical, pharmacological, and toxicological qualities directly from its molecular structure. The study of the quantitative structure–activity relationship is the name for this type of investigation (QSAR). Many chemical and biological features of chemical compounds under research can be predicted using topological indices [4].

2 Preliminaries

Definition 2.1 *The κ degree of any edge $\alpha\beta \in E(\Psi)$, denoted by $d_\kappa(\alpha\beta)$, is equal to the total number of vertices in the union of the α and β closed neighborhoods.*

Definition 2.2 *The degree of any vertex $\beta \in V(\Psi)$ is the sum of the degrees of all the vertices in its closed neighbourhood, i.e., ι the total quantity of edges incident to any vertices from the closed neighbourhood of β.*

3 Essential prerequisite

Some definitions of degree-based ι and κ K index ($K(\Psi)$), VL index ($VL(\Psi)$), Nirmala index ($N(\Psi)$), Albertson index ($A(\Psi)$) and Sombor index ($S(\Psi)$) are given bellow.

TI	κ degree based index	ι degree based index
$K(\Psi)$[17]	$k^{\kappa}(\Psi)=\sum_{e\in E(\Psi)}[d_{\kappa}(e)]^3$	$k^{\iota}(\Psi)=\sum_{e\in E(\Psi)}[d_{\iota}(e)]^3.$
$S(\Psi)$ [10]	$SO^{\kappa}(\Psi)=\sum_{\alpha\beta\in E(\Psi)}\sqrt{d_{\kappa}(\alpha)^2+d_{\kappa}(\beta)^2}$	$SO^{\iota}(\Psi)=\sum_{\alpha\beta\in E(\Psi)}\sqrt{d_{\iota}(\alpha)^2+d_{\iota}(\beta)^2}$
$VL(\Psi)$ [7]	$VL^{\kappa}(\Psi)=\frac{1}{2}\sum_{\alpha\beta\in E(\Psi)}d_{\kappa}(e)+d_{\kappa}(f)+4$	$VL^{\iota}(\Psi)=\frac{1}{2}\sum_{\alpha\beta\in E(\Psi)}d_{\iota}(e)+d_{\iota}(f)+4.$
$N(\Psi)$ [16]	$N^{\kappa}(\Psi)=\sum_{\alpha\beta\in E(\Psi)}\sqrt{d_{\kappa}(\alpha)+d_{\kappa}(\beta)}$	$N^{\iota}(\Psi)=\sum_{\alpha\beta\in E(\Psi)}\sqrt{d_{\iota}(\alpha)+d_{\iota}(\beta)}$
$A(\Psi)$[1]	$A^{\kappa}(\Psi)=\sum_{\alpha\beta\in E(\Psi)}\lvert d_{\kappa}(\alpha)^2-d_{\kappa}(\beta)^2\rvert$	$A^{\iota}(\Psi)=\sum_{\alpha\beta\in E(\Psi)}\lvert d_{\iota}(\alpha)^2-d_{\iota}(\beta)^2\rvert$

Table 1. Some of the ι degree based and κ degree based topological indices.

4 Research Aim

The K-index, VL-index, Nirmala index, Albertson index and Sombor index are some of the topological indices and polynomials of ι degree and κ degree based K-index, VL-index, Nirmala index, Albertson index and Sombor index are some of the primary aims of this article. Furthermore, the results of these indices have been developed to provide a better understanding of their behaviour.

5 Structure of copper oxide

Figure shows how the Cu_2O lattice formed in the $u\times v$ plane and accumulated in w layers. The vertices and edges of Cu_2O's crystal structure are $1+u+v+uv+w+uw+vw+6uvw$ and $8uvw$, respectively. Cu_2O vertices are divided into four divisions based on degrees: four vertices of degree zero, four vertices of degree one, four vertices of degree two, two vertices of degree three, two vertices of degree four, and two vertices of degree four. Similarly, Cu_2O edges are divided into $E_{(1,2)}$, which has $4(u+v+w)$ edges, $E_{(2,2)}$, which has $2(uv+uw+vw-2u-2v-2w+3)$ edges, and $E_{(2,4)}$, which has $8uvw-4uv-4uw-4vw+4u+4v+4w-4$ edges.

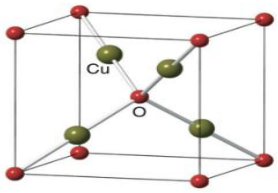

Figure 1: Cu_2O crystal structure

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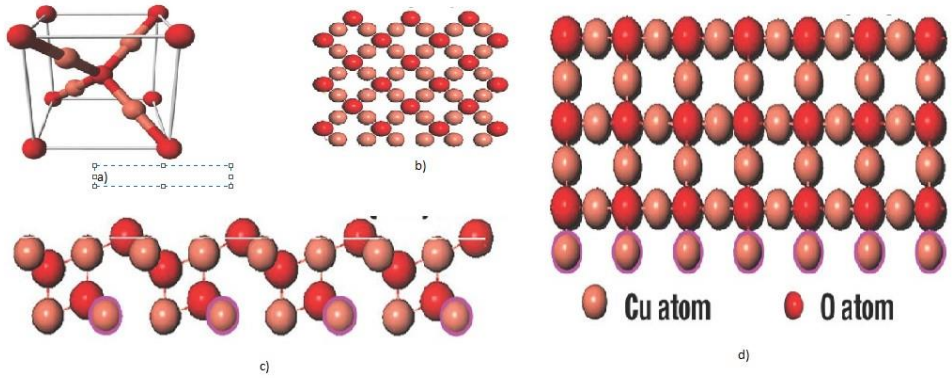

Figure 2: a)cuprite unit cell Cu_2O, b) Cu_2O crystal structure [1,0,0], c)Cu_2O crystal structure [1,1,1], d)Cu_2O crystal structure [1,1,0]

6 Main results

Theorem 6.1 *Let* Cu_2O *be a Copper(I) Oxide then* $F^{\kappa}(Cu_2O)$ *is*

$$F^{\kappa}(Cu_2O) = 716(u+v+w) - 736(uv+vw+uw) + 1728uvw - 696.$$

Proof. Assume Cu_2O be a Copper(I) Oxide. The edges are broadly divided into three types then total number of edges is $8uvw$. From the definition of each edge's end vertices κ degree can be used to calculate the degree of each edge, classified into three types which are given below.

$$E_1 = \{e \in E(Cu_2O) : d_{\kappa}Cu_2O(e) = 3\}$$

$$E_2 = \{e \in E(Cu_2O) : d_{\kappa}Cu_2O(e) = 4\}$$

$$E_3 = \{e \in E(Cu_2O) : d_{\kappa}Cu_2O(e) = 6\}$$

One can calculate easily that,

$$|E_1(Cu_2O)| = 4u + 4v + 4w - 8.$$

$$|E_2(Cu_2O)| = 2uv + 2uw + 2vw - 4u - 4v - 4w + 12.$$

$$|E_3(Cu_2O)| = 8uw - 4uv - 4uw - 4vw + 4u + 4v + 4w - 4.$$

$$F^{\kappa}(\Psi) = \sum_{e \in E(\Psi)} d_{\kappa}\alpha^3$$

$$\begin{aligned} F^{\kappa}(Cu_2O) &= ||E_1(Cu_2O)||(3^3) + ||E_2(Cu_2O)||(4^3) + ||E_3(Cu_2O)||(6^3). \\ &= 716(u+v+w) - 736(uv+vw+uw) + 1728uvw - 696. \end{aligned}$$

Theorem 6.2 *Let Cu_2O be a Copper(I) Oxide then*

1. $k^{\iota}(Cu_2O) = 18816(u+v+w) - 17472(uv+vw+uw) + 21952uvw + 1266.$
2. $SO^{\iota}(Cu_2O) = 80.941(u+v+w) - 56.087(uv+vw+uw) + 90.509uvw - 2.529.$
3. $VL^{\iota}(Cu_2O) = 320(u+v+w) - (224)(uv+vw+uw) + 320uvw - 24.$.
4. $N^{\iota}(Cu_2O) = 29.389(u+v+w) - 18.192(uv+vw+uw) + 32uvw + 0.8367.$
5. $A^{\iota}(Cu_2O) = 48(u+v+w) + 96(uv+vw+uw) + 96.$

Proof. Let cu_2o be a copper(I) oxide. The edges can be divided into five types and its total number of edges is $8uvw$. From the definition of each edge's end vertices ι degree can be used to calculate the degree of each edge, classified into five types which are given below.

$$E_1 = \{\alpha\beta \in E(Cu_2O): d_{Cu_2O}(\alpha) = 2, d_{Cu_2O}(\beta) = 5\}.$$

$$E_2 = \{\alpha\beta \in E(Cu_2O): d_{Cu_2O}(\alpha) = 4, d_{Cu_2O}(\beta) = 6\}.$$

$$E_3 = \{\alpha\beta \in E(Cu_2O): d_{Cu_2O}(\alpha) = 5, d_{Cu_2O}(\beta) = 8\}.$$

$$E_4 = \{\alpha\beta \in E(Cu_2O): d_{Cu_2O}(\alpha) = 6, d_{Cu_2O}(\beta) = 8\}.$$

$$E_4 = \{\alpha\beta \in E(Cu_2O): d_{Cu_2O}(\alpha) = 8, d_{Cu_2O}(\beta) = 8\}.$$

$|E_1(Cu_2O)| = 4u + 4v + 4w - 8$, $|E_2(Cu_2O)| = 2uv + 2uw + 2vw - 4u - 4v - 4w + 12$
$|E_3(Cu_2O)| = 4(u+v+w-2)$, $|E_4(Cu_2O)| = 2uv + 2uw + 2vw - 4u - 4v - 4w + 12$,
$|E_5(Cu_2O)| = 8(v-1)(u-1)(w-1).$

$$SO^{\iota}(\Psi) = \sum_{\alpha\beta \in E(\Psi)} \sqrt{d_{\iota}\alpha^2 + d_{\iota}\beta^2}$$

$$= |E_{(2,5)}| \sum_{\alpha\beta \in E_{(2,5)}(Cu_2O)} \sqrt{d_{\iota}\alpha^2 + d_{\iota}\beta^2} + |E_{(4,6)}| \sum_{\alpha\beta \in E_{(4,6)}(Cu_2O)} \sqrt{d_{\iota}\alpha^2 + d_{\iota}\beta^2}$$

$$+|E_{(5,8)}| \sum_{\alpha\beta \in E_{(5,8)}(Cu_2O)} \sqrt{d_{\iota}\alpha^2 + d_{\iota}\beta^2} + |E_{(6,8)}| \sum_{\alpha\beta \in E_{(6,8)}(Cu_2O)} \sqrt{d_{\iota}\alpha^2 + d_{\iota}\beta^2}$$

$$+ |E_{(8,8)}| \sum_{\alpha\beta \in E_{(8,8)}(Cu_2O)} \sqrt{d_{\iota}\alpha^2 + d_{\iota}\beta^2}.$$

$$= 80.941(u+v+w) - 56.087(uv+vw+uw) + 90.509uvw - 2.529.$$

We could use the same method to obtain results for the remaining indices.

Theorem 6.3 *Let Cu_2O be a Copper(I) Oxide then polynomials are given by*

1. $K^{`\iota}(Cu_2O, x) = (u+v+w)[4x^{125} - 4x^{512} + 4x^{1331} - 4x^{1728} + 8x^{2744}] + (uv+uw+vw)[2x^{512}2x^{1728} - 8x^{2744}] + 8uvwx^{2744} - 8x^{125} + 12x^{512} - 8x^{1331} + 12x^{1728} - 8x^{2744}$.
2. $SO^{`\iota}(Cu_2O, x) = (u+v+w)[4x^{5.38} - 4x^{7.21} + 4x^{9.43} - 4x^{10} + 8x^{11.31}] + (uv+uw+vw)[2x^{7.21} + 2x^{10} - 8x^{11.31}] + 8uvwx^{11.31} - 8x^{5.38} + 12x^{7.21} - 8x^{9.43} + 12x^{10} - 8x^{11.31}.$
3. $VL^{`\iota}(Cu_2O, x) = (u+v+w)[2x^{17} - 2x^{34} + 2x^{53} - 2x^{62} + 4x^{80}] + (uv+uw+vw)[x^{34} + 2x^{62} - 4x^{80}] + 4uvwx^{80} - 4x^{17} + 6x^{34} - 4x^{53} + 6x^{62} - 4x^{80}.$

4. $N^{`\iota}(Cu_2O,x) = (u+v+w)[4x^{2.64} - 4x^{3.16} + 4x^{3.60} - 4x^{3.74} - 8x^4] + (uv+uw+vw)[2x^{3.16} + 2x^{3.74} - 8x^4] + 8uvwx^4 - 8x^{2.64} + 12x^{3.16} + 12x^{3.74} - 8x^{3.60} - 8x^4.$
5. $A^{`\iota}(Cu_2O,x) = (u+v+w)[4x^{21} - 4x^{20} + 4x^{39} - 4x^{28} + 8x] + (uv+uw+vw)[2x^{20} + 2x^{28} - 8] + 8uvwx^{11.31} - 8x^{21} + 12x^{20} - 8x^{39} + 12x^{28} - 8.$

The proof method is as similar as theorem 2.

7 Numerical results

We offer mathematical conclusions which have been tied to the topological descriptors based on κ and ι degrees for the sub-atomic structures of cuprite oxide. We evaluated numerous u, v, and w estimations that were calculated using mathematical tables (Table 2). Many aspects of the understudied chemical molecule can be predicted using topological indices. Some of the graph invariants for instance K-index, Sombar index, VL-index, Nirmala index, and Albertson index that have been proposed for estimating the skeleton pertaining to the molecule of carbon spreading. A interesting field of research is still calculating the Undergraduate molecular graphs topological index based on degree.

So far, we have recorded numerically certain degree-based entropies for various u, v, w estimates for Cu_2O[u,v,w]. As the predictions of [u,v,w] are increments, you can see that all of the entropy values are in growing request [18].

$[u,v,w]$	$F^{\kappa}(\Psi)$	$k^{\iota}(\Psi)$	$SO^{\iota}(\Psi)$	$VL^{\iota}(\Psi)$	$N^{\iota}(\Psi)$	$A^{\iota}(\Psi)$
[1,1,1]	972	27250	162.54	584	329.59	528
[2,2,2]	8592	80114	534.12	1768	2494.03	1536
[3,3,3]	32532	291570	1655.28	5448	8389.31	3120
[4,4,4]	83160	793330	4069.16	13544	19935.45	5280
[5,5,5]	170844	1717106	8318.68	27976	39052.43	8016
[6,6,6]	305952	3194610	14946.95	50664	67660.26	11328
[7,7,7]	498852	5357554	24497.03	83528	107678.94	15216
[8,8,8]	759912	8337650	37511.95	128488	161028.47	19680
[9,9,9]	1099500	12266610	54534.79	187464	229628.84	24720
[10,10,10]	1527984	17276146	76108.60	262376	315400.07	30336

Table 2.Numerical depiction of estimated indices for various Cu_2O values.

8 Graphical Comparison of Cu_2O

In this portion we have depicted 3D graphs of polynomial of Cu_2O of various ι degree based topological indices.

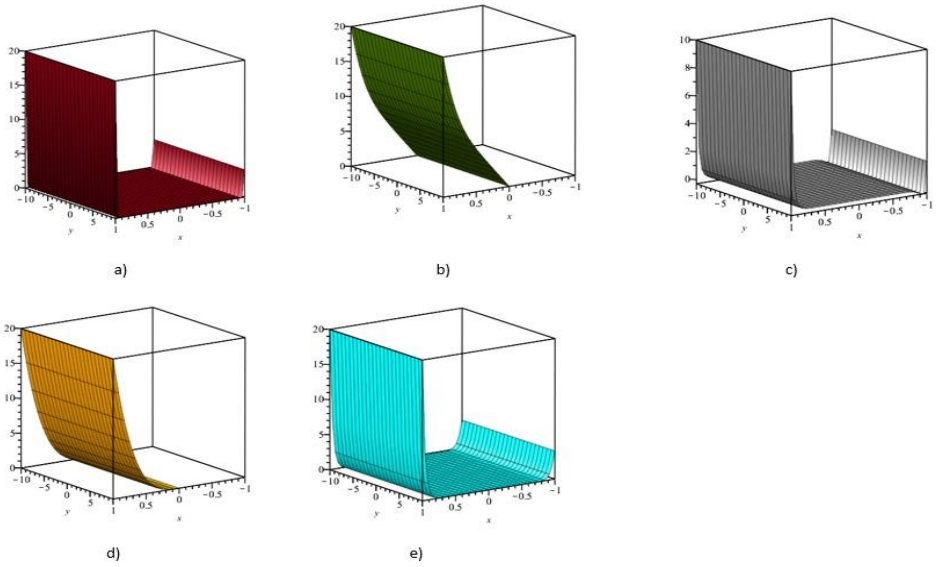

Figure 3: 3D graphs of polynomial of Cu_2O a)K edge index, b)sombor index, c)VL index, d)Nirmala index, e)Albertson index

9 Conclusion

The results of specific κ degree based and ι degree based indices of copper(I) oxide are presented in this article. Considering that the ι degree index has demonstrated a stronger prediction ability and correlation than standard degree-based indexes, according to the results of this study will assist researchers in better understanding the physical and chemical properties of copper(I) oxide.

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